Effect of Substrate Temperature on Optical Band Gap and Thickness of Spray Pyrolitically Deposited $CdZnTe_2$ Thin Films

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Abstract: ***Spray pyrolysis is a simple, inexpensive and economical method to produce a thin film on large substrate area. Semiconducting thin films of $CdZnTe_2$ have been deposited onto preheated glass substrate by varying substrate temperature from 250°C at an interval of 25°C to 325°C. The optimized deposition temperature is around 300°C.From optical transmission and reflection spectra, absorption coefficient(α) was calculated at various wavelengths ranging from 350 nm to 1100 nm and was of the order of 10^4 cm^{-1}.Band gap energy were determined from absorbance measurement in visible range using Tauc theory. It shows that the main transition at the fundamental absorption edge is a direct allowed transition. At the temperature of 300°C, the optical band gap is found to be 2.04 eV. At the temperatures less than or greater than 300°C, the optical band gap goes on increasing. The band gap energy value 2.04 eV- 2.13 eV is most suitable for many scientific studies and technological applications such as heat mirrors, transparent electrodes and solar cells. SEM study provide the information regarding the morphology of the material which confirms the formation of nano sized,nanotubes***

Keywords: $CdZnTe_2$ thin films, spray pyrolysis , optical band gap

1. Introduction

In the recent years much more attention has been paid in semiconducting II-VI compounds because of their optoelectronic properties and their possible applications in switching and memory devices, photodiodes and solar cells. The ternary compounds including Cadmium zinc telluride have attracted much more attention in the field of solar cells due to their interesting properties of band gap. For example, the band gap values of $CdZnTe_2$ ternary semiconductor was of 1.99 eV at substrate temperature 300°C. The evaluation of any material for application is complete and meaningful only when its structure and composition are precisely known. The reliability factor, which is the most important one for device application, can only be assured through a systematic and detailed study of the structural, electrical and zinc ditelluride is unit among II-VI series of semiconducting compounds as it shows both n- and p-type conductivity. The growth of ternary compound is a opens up the possibility of their application for novel optoelectronic devices such as light emitting diodes, photo electrodes, blue green lasers etc.[1] the visible region of electromagnetic radiation [2]. The research of the optical properties of CdZnTe system forms a basis of the active region of laser and LED. Most of the work has been done on $Cd_{1-x}Zn_xSe$ system. To the best of our knowledge, very less work has been reported on tellurium rich $CdZnTe_2$ polycrystalline material. Thus the present study is aimed at investing the optical band gap energies of $CdZnTe_2$ in the form of thin films at different substrate temperatures.

Several researchers studied properties in the II-VI semiconductor films using the variety of methods such as flash evaporation, chemical vapour deposition, r.f. sputtering, chemical bath deposition, electrodeposition [3-5] and spray pyrolysis [6-7].

We have chosen spray pyrolysis due to simple, inexpensive and produce a thin film on large substrate area and it is suitable for scientific studies and for many technological and industrial applications. The advantage of the technique is that just by varying the concentration of precursor and substrate temperature, it is possible to control stoichiometry of the deposits. The present study deals with the effect of substrate temperature on optical band gap and thickness of spray pyrolitically deposited $CdZnTe_2$ thin films.

2. Experimental Details

Aqueous solutions of cadmium chloride, zinc chloride and tellurium tetrachloride of 0.02 M of each were prepared in double distilled water. Chemicals used were of AR grade. The solutions are mixed in one in the proportion 1:1:3.2 by volume. The film shows a tellurium deficiency [8-9] if the ratio of proportion of solution was taken as 1:1:2 by volume. In order to find optimized condition for deposition of $CdZnTe_2$ thin films, the deposition was carried out by varying one of the parameters as substrate temperature and keeping others at fixed value.

Sprayer was mechanically moved to and fro to avoid the formation of droplets on the substrate and insure the instant evaporation from the substrate. The distance between the sprayer nozzle and substrate was kept at 30 cm. The spraying was done in the atmosphere at the spray rate 3.5 ml/min. with a maintaining pressure of 12 Kg/cm^2. The temperature of substrate was maintained at 250°C,375°C,300^0C,325°C and was measured by pre-calibrated copper constantan thermocouple. The thicknesses of the films were measured by weighing method on unipan microbalance and Michelson interferometer. The thicknesses of the films found by both the methods were found to be approximately same. The difference was of the order of 0.003 µm. Optical transmittance and reflectance was taken on UV-1800-Shimandzu Spectrophotometer in the wavelength range 350 nm to 1100 nm.

3. Results and Discussion

In spray pyrolysis technique aqueous solutions of required material are mixed in proper proportion and then sprayed onto preheated substrate. When droplets of sprayed solution reach the hot substrate, owing to pyrolytic decomposition of the solution, well adhered and good quality films are formed on the surface of the substrate.

3.1 Thickness variation

The thickness of $CdZnTe_2$ thin films deposited at various substrate temperatures was measured and the graph was plotted between the thickness of the films and substrate temperature as shown in fig.1

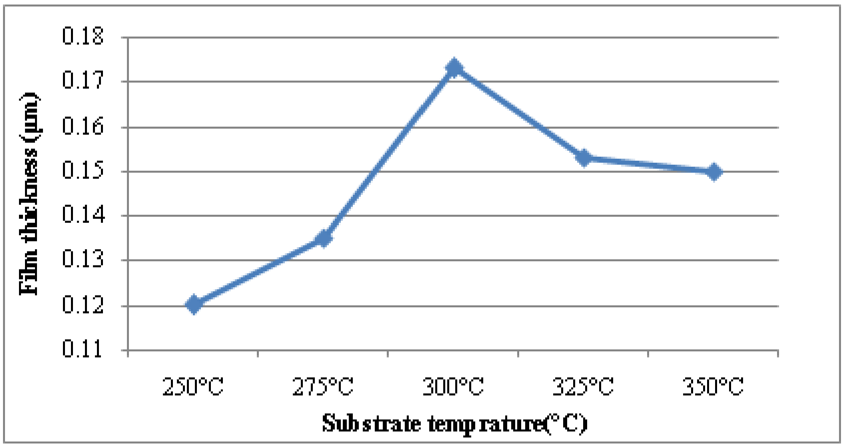

Figure 1: Variation of film thickness of $CdZnTe_2$ thin films with substrate temperature

Graph shows that the thickness of the as deposited $CdZnTe_2$ thin films increases with temperature, attains the maximum value at 300°C and then decreases with further increase in substrate temperature. At low temperatures (<300°C), the temperature may not be sufficient to decompose the sprayed droplets from the solution and hence the deposits results into low thickness. At substrate temperature 300°C, deposition occurs at optimum rate resulting in terminal thickness of 0.1730µm. At higher substrate temperatures (>300°C) film thickness decreases due to higher evaporation rate of initial ingradients[10].

3.2 Optical study

The optical transmission spectra of $CdZnTe_2$ thin films deposited at different substrate temperature was taken on UV-1800-Shimandzu spectrophotometer in the wavelength range 350 nm to 1100 nm. Fig.2. Shows the transmission versus wavelength of as deposited $CdZnTe_2$ thin films at different substrate temperatures.

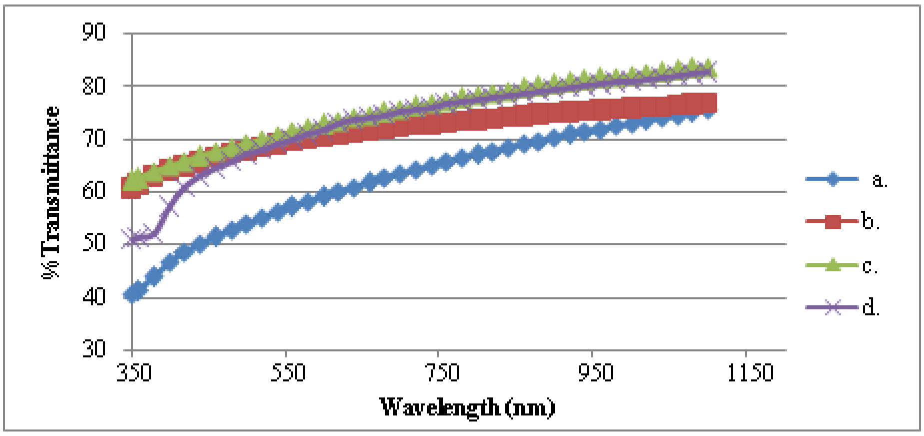

Figure 2: Transmission spectra of $CdZnTe_2$ thin films deposited at substrate temperature of a)250°C, b)275°C, c)300°C, d)325°C.

It was observed that onset of decrease of transmission gives the optical absorption edge. The optical coefficients were calculated for each wavelength given by relation,

$$\alpha = 1/t \ln(1/T) \quad (1)$$

Where, t- thickness of the films, T- transmittance of the film.

An analysis of the spectrum showed that the absorption at the fundamental absorption edge can be described by the Taue relation [11],

$$\alpha = (A/h\nu)\,(h\nu\text{-}E_g)^n \qquad (2)$$

Where hv –photon energy, A-constant which is different for different transitions, n = 1/2 for direct allowed transition and n = 2 for indirect allowed transition.

To calculate the exact value of band gap, a graph is plotted between $(\alpha h\nu)^2$ versus hv of as deposited thin film of $CdZnTe_2$ thin film at differentsubstrate temperatures as shown in fig.3.

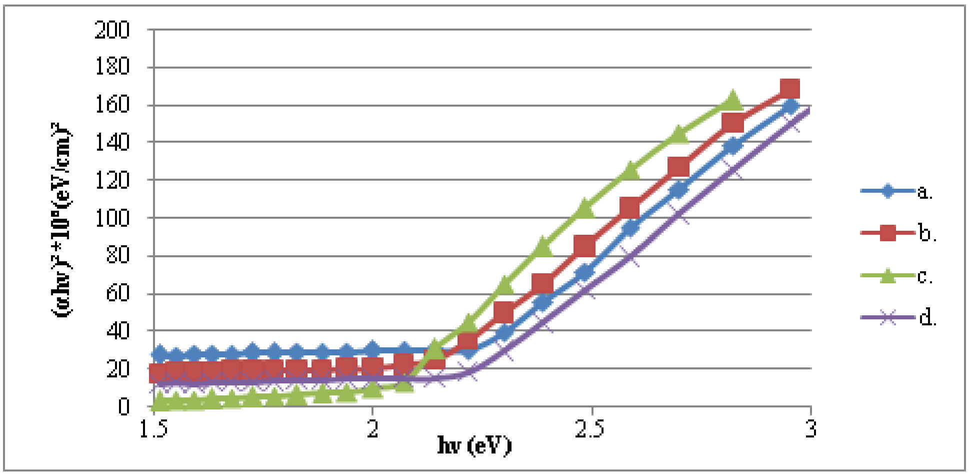

Figure 3: Variation of(αhν)² in (eV/cm)² versus hν in eV for as deposited $CdZnTe_2$ thin film deposited at different substrate temperatures a)250°C,b) 2750°C,c)300°C,d)325°C

The linearity of each graph showed the direct allowed transition, indicating the semiconducting nature of the films. The linear portion of the plot was extrapolated to meet on hv axis yield, the value of band gap energy was found to be 2.04 eV. These results are well agreed with the Alex Zunger et.al [12]. They have reported the band gap value of 1.98 eV by modern epitaxial growth technique. M. Bilal Faheem et.al [13] have also reported optical band gap value vary from 1.48 to 2.26 eV.of $Cd_{1-x}Zn_xTe$ thin films by varying the Zn content prepared by thermal evaporation technique. The optical transmission spectrum of the films under study shows that the transmission spectra mechanism is due to the direct allowed transition .Our calculated value of optical band gap 2.04 eV are less than the value reported as 2.2748 to 2.2226 eV by M. Becerril et.al.[14] by r.f. sputtering method to prepare Zn rich $Zn_{1-x}Cd_xTe$ thin films on 7059 corning glass substrate at room temperature. This shows that spray pyrolysis produce a good stoichiometric in semiconducting nature. The linear plot of $(\alpha h\nu)^2$ versus hv over wide range of photon energies shows $CdZnTe_2$ thin film has a direct allowed transition.

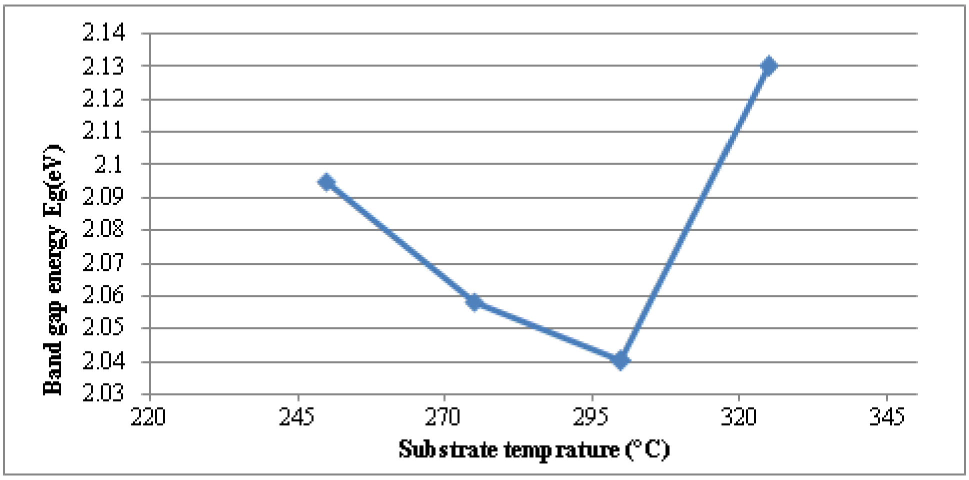

Figure 4: Variation of optical band gap energy (E_g) with substrate temperature of as deposited $CdZnTe_2$ thin films

From fig.4 it is observed that optical band gap energy of $CdZnTe_2$ thin film is 2.04 eV at substrate temperature 325°C. The band gap energies determined for the samples decreases from2.13 to 2.04eV with increase in substrate temperature upto 300°C and it further increases with increase in substrate temperature. This shows that 300°C is the most suitable substrate temperature for depositing $CdZnTe_2$ thin film with optical band gap value which is most suitable for many scientific studies and technological applications, such as sensors, heat mirrors, solar cells transparent electrodes and piezoelectric devices.

4. Conclusion

Spray pyrolysis is a simple and inexpensive method to produce a thin film. Optical band gap of $CdZnTe_2$ thin film was of 2.04 eV at 300°C substrate temperature which was calculated from $(\alpha h\nu)^2$ versus (hν) plot. The plot of optical band gap energies vs. substrate temperature is parabolic in nature which shows that at substrate temperatures less than or greater than300°C,band gap energy values goes on increasing. The linearity of the plot shows the direct allowed transition.

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