Study of Variation of Band Gap Energy and Thickness with Temperature of $Cuinte_2$ Thin Films Prepared by Spray Pyrolysis

Physics

KEYWORDS : Spray pyrolysis, CuInTe2 thin films

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ABSTRACT

Spray pyrolysis is a simple and inexpensive method for preparation of thin films on a large area. CuInTe2 thin films were prepared by spray pyrolysis on glass substrate temperatures between 2750c to 3750c at interval of 250c. thicknesses of the optical band gap energy were calculated by Michelson interferometer. Optical band gap energy were calculated by plotting the graph between (αhv)2 vs hv. The study reveals that CuInTe2 is direct band gap energy equal to 0.98 eV which matching with single crystal. Band gap energy decreases as temperature increases upto 3500c. Further increase in temperature the band gap energy increases while increase in temperature thickness of the films increases upto 3500c. After this decrease of thickness takes place. The band gap at temperature 3500c confirms the stability of materials with nearly stoichiometry

Introduction: -

The I-III-VI2 group material, ternary chalcopyrite compound is the leading semiconductor material due to low cost and abundance of the constituent element. These group of compound are most promising candidates for application such as photo-voltaic power generation system because a) are direct band gap semiconductors with high absorption coefficient b) can be easily obtained in the thin films form, Either n- type or p-type c) have energy band gap (1-2 eV) in the optical range for solar energy conversion d) have lattice constant which matches that of CdS, widely used in solar cell technology. The highest conversion efficiency of 19.9% was demonstrated for Cu(In, Ga) Se2 based thin films solar cells with small area (<cm2) [2]. The characterization of CIS thin films depends on native defects such as deviation of stoichiometry deviation during fabricating CIS thin films is required. Large single crystals of CIT, free from voids and micro cakes, have been obtained mainly by programmed directional freezing (PDF) and vertical Bridgman technique [3, 4]. This material is normally found to be p- type conducting. There is report in the literature where n-type CIT is produced by prolonged annealing of very thin sample in the presence of Indium [5]. Also p- type sample of CIT grown by the closed tube chemical vapor transport technique when later heat treated in Cd atmosphere and thin films annealed in vacuum are found to have n-type behavior. No change in the conductivity type is observed [4]. Cu-III-VI2 thin films have been deposited using various technique; electroplating technique sputtering [6], molecular beam epitaxy [7], sputtering technique [8], flash evaporation [9] and electro deposition [10].

We have chosen the economical and convenient method of chemical spray pyrolysis for the deposition of thin films. Typical spray pyrolysis equipment consist of an atomizer, precursor solution, substrate, heater and temperature controller.

We have deposited CuInTe2 thin films by this method and study the effect of temperature on thickness and optical band gap of the thin films. Thickness of the thin films was measured by Michelson Interferometer. We have used Shimazdu UV-1800 spectrophotometer to measure the optical transmission of the different substrate temperature was measured by pre-calibrated copper-constantan-thermocouple.

Experimental Details:-

An aqueous solution of copper chloride, Indium tri-chloride and tellurium tetra-chloride of 0.02 M of each were prepared in double distilled water. The deposition was carried out onto commercially available glass substrate of the size (7.5×2.5×0.1) cm3. The analytical reagent grade chemicals were used. For preparing CuInTe2 thin film, we have mixed each solution in the ratio 1:1:3.2 by volume. Excess tellurium is necessary to obtain CuInTe2 the temperature of the substrate measured by a pre-calibrated copper constantan thermocouple was maintained and vary from 2750c to 3750c at the difference with 250c. The spray rate of 3.5 ml/min was maintained. The distance between the sprayer nozzle and substrate was 30 cm. The glass sprayer was mechanically moved to and fro during spraying to avoid the formation of droplets on the hot substrate and to ensure instant evaporation. The optical band gap was estimated by measuring optical transmission on Shimazdu UV-1800 spectrophotometer. The thickness of the films was measured by Michelson interferometer.

Optical absorption:-

Optical transmission studies of CuInTe2 thin films prepared at different temperature were carried out in the wavelength range 350 to 1100 nm at room temperature as shown in fig. 1. The absorption coefficient (α) at various wavelengths for the sample thickness (t) is given by,

$$\alpha = 1/t \log (Io/I) \qquad (1)$$

where, Io and I are the intensities of incident and transmitted radiation respectively.

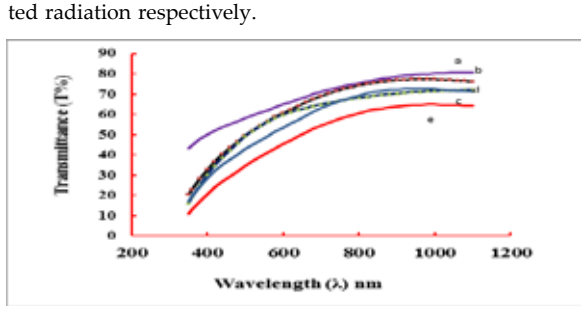

Figure 1. Wavelength(λ) Transmittance with different temperature of the films a) 275 0C, b) 300 0C, c) 325 0C d)350 0C, e) 375 0C

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The absorption coefficient (α) at various wavelengths was calculated from the transmission curve for different temperature. Plotting the graph between $(\alpha h\nu)^2$ against $h\nu$ for different temperature as shown in fig 2. The linear portion of each was extrapolated to meet energy ($h\nu$) axis given the value of band gap E_g.

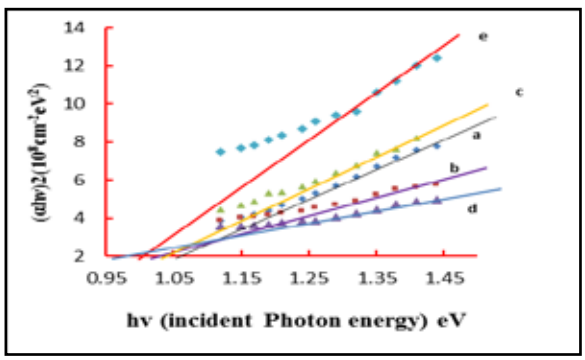

Figure 2. $(\alpha h\nu)^2$ vs photon energy of different temperature of thin films a) 275 ^{0}C, b) 300 ^{0}C, c) 325 ^{0}C d)350 ^{0}C, e) 375 ^{0}C

The band gap energy value for different samples decrease from 1.05 eV to 0.98 eV with increase in substrate temperature upto 3500c and further increase in substrate temperature, the band gap energy at 3500c of the crystalline material confirms the stability of material with nearly stoichiometry. The minimum band gap energy of the crystalline material at 3500c confirms the stability of the material with nearly stoichiomtry the variation of band gap energy with substrate temperature is shown in fig 3. This is in good agreement with published by authors [6, 11]; they reported band gap energy 0.93 to 1.06 eV for CuInTe2 thin films. This result was in good agreement with results reported by Sawant and Bhosale [12] and tembhurkar et al [13] for spray pyrolytically deposited CdInS4 thin films

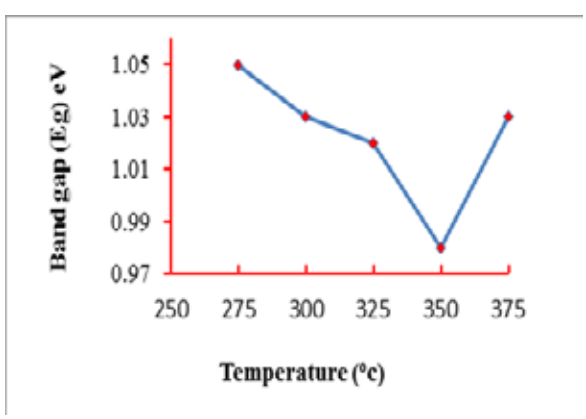

Figure 3. Temperature vs Band Gap (Eg)

Thickness Variation:-

The thickness of the films deposited at various substrate temperatures was measured by Michelson Interferometer. The variation of thickness with substrate temperature is shown in fig. 4. It was observed from fig. 4 that the thickness of the films was increases with increase in temperature and attains the maximum value at 3500c and decreases for further increase in temperature. The deposition occurs at optimum rate at temperature 3500c. At lower temperature < 3500c the temperature may not be sufficient to decompose the sprayed droplets and substrate [12]. At higher substrate temperature > 3500c, the film thickness decrease due to higher evaporation rate of the initial ingredient [14].

Table 1.Shows the thickness and band gap with temperature

Sr.No	Temperature (0c)	Thickness (t) µm	Band gap (E_g) eV
1	275	0.1240	1.05
2	300	0.1530	1.03
3	325	0.1730	1.02
4	350	0.2030	0.98
5	375	0.1820	1.03

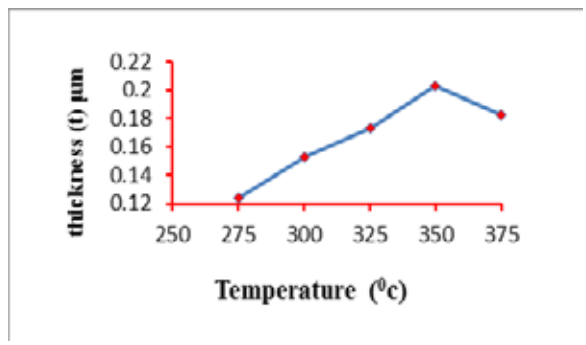

Figure 4. Temperature vs Thickness (t)

Conclusion:-

In conclusion it is established that CuInTe2 thin film of good quality with stoichiometry close to 1:1:2 can be prepared by spray pyrolysis method the film deposited at optimized substrate temperature of 3500c and concentration of 0.02 M are polycrystalline having energy band gap 0.98 eV. The observed variation in band gap energy for CuInTe2 films with deposition temperature is due to corresponding variation in particle size and film thickness with deposition temperature.

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