Temperature Effect on Structural Properties of Copper Indium Telluride Thin Films

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Abstract: CuInTe₂ thin films prepared by spray pyrolysis by using aqueous solution copper chloride, Indium trichloride and Tellurium tetrachloride of 0.003 M of each. From the XRD diffraction pattern, the crystallinity size of the films were calculated from the preferential peak (200) plane found to be maximum at optimised temperature 350°C. XRD study reveals that CuInTe₂ thin films cubic in nature with preferred orientation along 200 plane.

Keywords: CuInTe₂ thin films, XRD study.

I. Introduction

I-II-VI compounds, especially copper-chalcopyrite thin films have played a major role in the films. Photo-voltaic technology. Typical copper-chalcopyrite-based absorber materials are CuInS₂, CuInSe₂, CuGaSe₂, Ga₃GaS₂ and their alloys with the band gap 1.05-1.7 eV, which is favorable for the solar cells. Among them CuInTe₂ is one of most popular ternary chalcopyrite semiconductor that have attracting interest for its direct band gap value in the range between 0.92 and 1.06 eV which make them quite interesting for solar energy conversation. Polycrystalline thin films of CuInTe₂ are usually crystallized in cubic structure with lattice constant a=6.080 Å and in the tetragonal structure with lattice constant ‘a’=6.194 Å and ‘c’=12.415 Å. CuInTe₂ thin films is more environment friendly than CuInSe₂ and CuGaSe₂ thin films due to toxicity of selenium. There are different method to prepare thin films, such as, r.f. sputtering, flash, vacuum evaporation, and chemical vapour deposition including novel photochemical deposition, Ion layer gas reaction and spray pyrolysis (1-3).

We have chosen spray pyrolysis due to simple, inexpensive, easy to handle and to prepare on large substrate area. In this method, composition of the constitution can be easily varying in the spray solution. Spray pyrolysis deposition method is a scalable process and it is used for depositing large area films, which are essential for photo-voltaic application.

In the present work, CuInTe₂ thin films were deposited by spray pyrolysis method in an air atmosphere on glass substrate between temperature 300°C-350°C and studied the effect of temperature of a structural properties.

II. Preparation Of The Sample

Thin films of CuInTe₂ have been prepared by using aqueous solution of copper chloride, Indium trichloride and Tellurium tetra-chloride. Molarity of each solution was taken as 0.003 M. These solution are mixed in one by taking proportion of solution is 1:1:3 by volume. Tellurium deficiency (4,5) was observed if the solution proportion taken 1:2:2 by volume. The biological glass slide used as a substrate. Temperature of the substrate was varied from 300°C to 375°C in the interval of 25°C. Detailed experimental technique was given elsewhere (4,5). Temperature of the substrate was measured by pre-calibrated copper constantan thermocouple. Thickness of the films was calculated by Michelson interferometer. X-ray diffraction pattern were taken on Philips X-ray diffractometer using Cuku-radiation of wavelength λ=1.452 Å.

III. Structural Properties

Fig.1. a,b,c, and d represent X-ray diffraction pattern of as deposited at temperature 300°C, 325°C, 350°C and 375°C.

Fig. 1. X-ray pattern of as deposited CuInTe2 thin film prepared at temperature a) 300°C, b) 325°C, c) 350°C and 375°C.
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From X-ray diffraction data, $d_{hkl}$- interplanar spacing was calculated using the bragg’s relation.

\[ 2d_{hkl}\sin \theta = n\lambda \]  \hspace{1cm} (1)

Where $\lambda$-be the wavelength of X-ray used (1.542Å) $\theta$-be diffracting angle $n$-be the order number.

The lattice constant of cubic structural of CuInTe$_2$ thin films was calculated by using relation,

\[ 1/d^2 = h^2+k^2+l^2 / a^2 \]  \hspace{1cm} (2)

The crystallite size of the films was calculated from the X-ray diffraction data using Full width of half maxima and Debye-scherrer formula,

\[ D = 0.9\lambda / B \cos \theta \]  \hspace{1cm} (3)

Where B- is the full width of half maxima peak in radian.

\( \theta \)-be the Bragg’s diffraction angle at peak position in degrees.

Observed diffraction peaks of CuInTe$_2$ thin films at 20 values of angles 25.30, 29.41 , 49.75, 51.99, 60.76, 69.00 & 77.01 corresponding to the lattice planes (111), (200),(220), (311), (222), (400), (420), & (422) respectively. Each peak in the diffraction pattern were indexed and the corresponding interplanar spacing $d$ values were calculated. They are compared with the JCPDS Data values (6). The height of the each peaks increases and some new peaks beings to appears when preparation temperature increases from 300°C to 350°C.

But when preparation temperature of the films at 375°C, the height of the preferential orientation of the peak (200) slightly decreases. Therefore preparation of thin films kept at 350°C is fixed for all the films. The films deposited at temperature 350°C have good crystallite and it well adherent to the substrate (7). The films prepared below 350°C are found to poor crystallized. Our calculated 20 values of each diffraction peak are well agree with mahalingam etal. (7) for electroplated copper Indium Telluride thin films. Similar behaviour was also noted by mahalingam etal. (8) for ZnHgTe thin films.

The crystallite size calculated using maximum intensity peaks (200) plane are 25 nm, 34 nm, 60 nm,& 40 nm for the films prepared at temperature 300°C, 325°C, 350°C and 375°C. It was observed that if the preparation temperature of the films increases, crystallinity size also increase up to the optimised temperature 350°C. After increases the temperature (375°C), the crystallinity size decreases. Our Calculated results are well agree with other workers (6, 7)

IV. Conclusion

CuInTe$_2$ thin films were deposited at different substrate temperature by spray pyrolysis method. From the X-ray study, the crystalline size of the films were calculated, it shows that crystalline size increase when temperature increases and it is maximum at optimised temperature (350°C). Structural studies shows that the deposited films is cubic in nature with preferred orientation along (200) direction.

Acknowledgment

Author would like to express his thanks to U.G.C. for financial support in the form of major research project. Author also thanks to principal of my, S.K. Porwal college Kamptee for provident the research facility in the physic department.

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