Growth and Characterizations of Nanostructured Cu_{0.75}In_{0.25}Se Thin Films

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ABSTRACT

 $Cu_{0.75}In_{0.25}Se$ thin films were deposited by thermal evaporation technique above the glass substrates. The phase purity and microstructure were analyzed by scanning electron microscopy. The investigations show that grown thin films were polycrystalline in nature having monoclinic crystal structure. Analysis of the optical transmittance spectra of $Cu_{0.75}In_{0.25}Se$ thin films yields a value of 2.0 - 2.8eV for the fundamental band gap.

Keywords: XRD, SEM, EDAX, UV-VIS Spectroscopy.

1. INTRODUCTION

The ternary compound CuInSe is known for their suitability in PV devices due to the higher absorption coefficient [1, 2]. CuInSe is considered as a promising absorber material for thin film solar cells [3]. The important requirements for the efficient performance of these devices should be crystallinity and compositional balance. There is various deposition techniques have been executed for the growth of CuInse thin films: molecular beam epitaxy [5, 6] pulse laser deposition [7], spray pyrolysis [8], RF sputtering [9], CBD [10]. Thermal evaporation is one of the important methods for the deposition of compound materials because of, informality and reproducibility. We have deposited CuInSe thin films by a thermal evaporation method by feeding source material onto molybdenum boat. This procedure of allowing a very small quantity of the material into the boat and evaporation to completion is repeated to get films with required thickness. In spite of these precautions other deposition parameters involved such as source to substrate distance, deposition rate and substrate temperature. These growth parameters lead to variation in structural, optical and electrical properties. Hence, it is necessary to study the properties with respect to the deposition parameters. In this paper, we report on the results of XRD and SEM investigations of structural properties of CuInSe thin films. Further, the result analysis and optical property studies are also presented.

2. EXPERIMENTAL DETAILS

The ternary alloy of $Cu_{0.75}In_{0.25}Se$ was made by melt quench method. The pure mixture of Copper, Indium and Selenium was kept in evacuated quartz tube and heated at about 1000 °C for 24 hours and then quenched in ice cooled water. The films of $Cu_{0.75}In_{0.25}Se$ were grown by thermal evaporation technique under pressure of 10^{-5} torr. The source to substrate distance was kept about 14 cm. The samples of different thicknesses were deposited under similar conditions. The thickness of the films was monitored on Digital Thickness Monitor (DTM-101) provided by Hind-Hi Vac. The deposition rate was maintained 8-10 Å/sec for every sample preparation. Before evaporation, the glass substrates were cleaned throughout using chromic acid, detergent and acetone.

3. RESULTS AND DISCUSSIONS

3.1. XRD Analysis

The crystal structure and its other parameters can be studied by XRD pattern. The XRD patterns of grown $Cu_{0.75}In_{0.25}Se$ thin films were obtained by using the Bruker having $CuK\alpha$ radiation. The sample of $Cu_{0.75}In_{0.25}Se$ was scanned in the 2 θ range of 0° to 80°. Figure 1 shows the XRD patterns of $Cu_{0.75}In_{0.25}Se$ thin films having thickness 3000 Å.





From XRD pattern the peaks are found at 2θ peaks 25.0° , 27.5° , 30.5° , 39.9° and 44° having hkl plans (202), (423), (134), (035) and (304) are observed respectively. The plans of reflections are good agreement with JCPDS data. The multiple peaks are observed. It shows the material is polycrystalline in nature [11]. The major peak is observed at 25° belongs to monoclinic shape. The average crystal size (D) was calculated by using the Scherrer formula:

$D = 0.94 \lambda / \beta \cos \Theta$

Where, λ is the wavelength of X-ray, β is Full Width Half Maxima, θ is the diffraction angle. The crystal size was found to 425 nm. The unit cell parameters a, b and c are found to be 15.47, 17.21 and 15.36 respectively.

3.2 SEM Analysis

The surface morphology can be studied by Scanning Electron Microscopy (SEM) analysis. The SEM analysis was done with help of FESEM (Zeiss EVO50). Figure 2 shows the SEM image of Cu_{0.75}In_{0.25}Se thin film. From the SEM images it can be seen that the grown samples are homogeneous [12, 13]. The grains are uniformly distributed all over the area of the substrate. The nano grains are closely packed together. The nano grains forms cluster in somewhat granular shaped [14-15]. The average cluster size is found about 12 nm for both samples. The samples are free from microscopic defects like cracks or peeling off. The surfaces of the films were sufficiently flat.



Fig. 2 SEM Photographs of the Cu_{0.75}In_{0.25}Se Thin Film





The presence of elements can be detected by using EDAX analysis. The figure 3 shows the EDAX pattern of $Cu_{0.75}In_{0.25}Se$ thin film. The present elements were detected at KeV with atomic percentages of 0.07%, 48.65% and 51.27 %. There is no evidence found of any type of impurities. It proves the purity of grown sample. The presence of other peaks are due to the glass substrate and gold coating during the characterizations.

3.4 UV – VIS Spectroscopy

The optical properties like absorbance transmittance of grown $Cu_{0.75}In_{0.25}Se$ thin film were studied by using UV – VIS Spectroscopy. The optical absorption patterns were obtained within the 400 – 800 nm wavelength ranges by using UV – VIS Spectrophotometer.



Fig. 4: Absorbance Spectra of Cu_{0.75}In_{0.25}Se Thin Films



Fig. 5: Transmittance Spectra of Cu_{0.75}In_{0.25}Se Thin Films

Figure 4 and 5 shows the absorbance and transmittance patterns of grown $Cu_{0.75}In_{0.25}Se$ thin films respectively. The higher absorbance is noticed within the 425-475 nm wavelength regions. The $Cu_{0.75}In_{0.25}Se$ thin films with various thicknesses have good absorbance. Hence the $Cu_{0.75}In_{0.25}Se$ can be used as absorber material in fabrication of solar cell. The optical band gap of grown thin films has been calculated by Tauc relation:

$\alpha hv = A (hv - Eg)^n$

Where, α is the absorption coefficient, hv is the photon energy, Eg the band gap. The optical band gap of the grown Cu_{0.75}In_{0.25}Se thin films were determined from a plot of $(\alpha h\nu)^2$ Vs Eg [16] as shown in Figure 6. The Cu_{0.75}In_{0.25}Se is a direct band gap material. The band gap values were obtained as 2 to 2.8 eV. The Cu_{0.75}In_{0.25}Se can be used in solar cell fabrication.



Fig. 6: Optical band gap of Cu_{0.75}In_{0.25}Se Thin Films

CONCLUSION

The XRD study illustrates the formation of polycrystalline $Cu_{0.75}In_{0.25}Se$ thin film having monoclinic crystal structure. The SEM revels that grains are spherical in shape and uniform distribution over the substrate. The presence of elemental constituents was confirmed with the help of EDAX spectrum. The optical band gap of the sample varies from 2.0 to 2.8 eV which can be used for efficient photo voltaic devices.

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