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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.13, pp 5408-5411, November 2014

MESCon 2014 [4th -5th September 2014]
National Conference on Material for Energy Storage and Conversion- 2014

# Structural, Morphological and Optical Properties of Copper Selenide Thin Films

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**Abstract:** Thin films of copper selenide have been deposited on indium doped tin oxide coated glass substrates. X-ray diffraction analysis revealed that the deposited films possess polycrystalline in nature. Optical absorption analysis showed that the deposited films possess band gap value around 2.1 eV.
**Keywords:** Metal Chalcogenides, CuSe; Thin Films, Electrodeposition, X-ray diffraction.

## Introduction

Copper Selenide (CuSe) is a direct band gap p-type semiconductor with an energy gap value in the range between 2.1 and 2.7 eV which make them interesting for solar energy conversion[1]. Copper Selenide has many structural phases such as α-$Cu_2Se$, $Cu_3Se_2$, CuSe and $CuSe_2$ in stoichiometric form and $Cu_{2-x}Se$ phase in non-stoichiometric form[2]. Thin films of CuSe are normally crystallized in hexagonal structure and orthorhombic structure. Numerous techniques have been used to obtain CuSe thin films viz., thermal evaporation[3], vacuum evaporation[4], solution growth technique[2]and chemical bath deposition[5]. Among them, electrodeposition technique provides many advantages over vacuum and other processes, such as low temperature growth, control of film thickness and morphology, potentially low capital cost, etc.[6]. In this paper, thin films of CuSe have been prepared on indium doped tin oxide (ITO) coated glass substrates using electrodeposition technique. Deposited films are subjected to X-ray diffraction, Scanning electron microscopy and Optical absorption analysis, respectively. The experimental observations are discussed in detail.

## Experimental

CuSe thin films were deposited on ITO substrate (sheet resistance 20Ω/❑) from an aqueous electrolytic bath containing 0.05 M $CuSO_4$ and 0.005 M $SeO_2$. The electrochemical experiments were carried out using a Potentiostat/Galvanostat (BioLogic-SP50, France) employing three electrode configuration with ITO substrate as working electrode, graphite plate as counter electrode and saturated calomel electrode (SCE) as reference electrode, respectively. The solution pH and deposition potential were maintained at 2.0 ± 0.5 and -800 mV versus SCE.Thickness of the deposited films was estimated using weight difference method. X-ray diffraction data of the deposited films was recorded using an X-ray diffractometer (XPERT PRO ANALYTICAL X-ray diffractometer, Netherland). Surface morphology was analyzed using Scanning electron microscope (Philips,

Model XL 30). Optical absorption analysis of the deposited films was recorded using and UV-Vis-NIR spectrophotometer (Shimadzu Model 2600, Singapore).

## Results and Discussion

### Film Thickness

Thickness of the deposited films is measured using weight difference method. Thickness value of films obtained under optimized condition at various deposition time is given in Table 1. It is observed from table that value of film thickness increases with deposition time and reaches its maximum value at a deposition time of 40 minutes. Further increasing deposition time thickness value decreases which is not given in table. Hence, films with maximum thickness value are obtained at a deposition time of 40 minutes.

**Table 1. Variation of structural parameters with deposition time for CuSe thin films**

| Sl.No | Deposition Time (minutes) | Film Thickness (nm) | Crystallite Size, D (nm) | Strain, ε $(lines^{-2}/m^4)x10^{-3}$ | Dislocation Density, δ $(lines/m^2)x10^{14}$ |
|---|---|---|---|---|---|
| 1 | 20 | 455 | 34.3 | 1.712 | 8.455 |
| 2 | 30 | 585 | 35.8 | 1.634 | 7.766 |
| 3 | 40 | 785 | 43.4 | 1.350 | 5.299 |

### Structural Properties

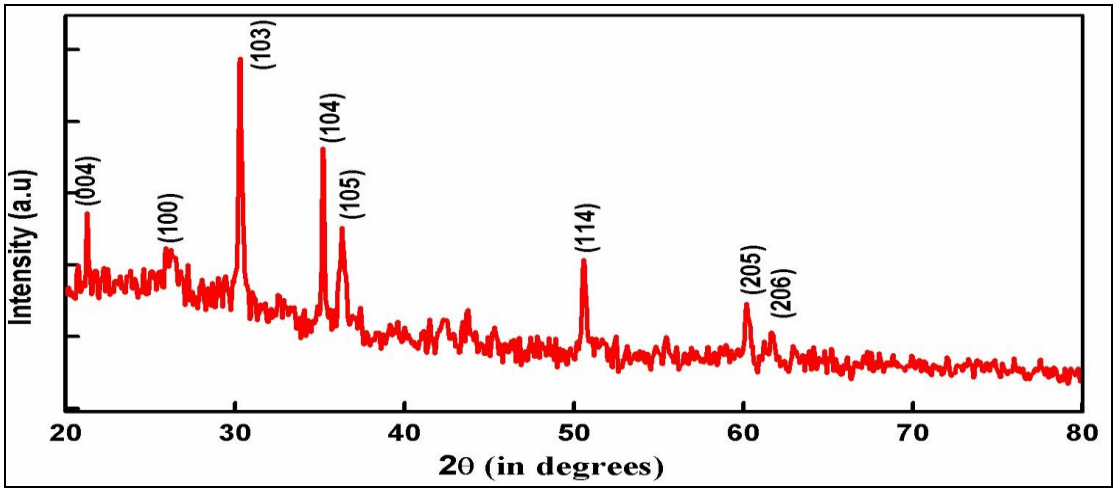


**Figure 1. XRD pattern of CuSe thin films obtained at a deposition time of 40 minutes.**

X-ray diffraction pattern of CuSe thin films obtained at a deposition time of 40 minutes is shown in Fig.1. XRD patterns indicated that the deposited films possess polycrystalline in nature with hexagonal structure with lattice constants (a=3.948 Å; c= 17.285 Å). The different peaks in the diffractogram is indexed and the corresponding values of interplanar spacing "d" is calculated and compared with standard JCPDS ICDD file for hexagonal CuSe[7]. The height of (103) peak is found to be higher than all other peaks in the XRD pattern indicated that the crystallites are preferentially oriented along (103) plane. The value of crystallite size is determined using Debye Scherrer formula which is given in Eq. (1)[8]

$$D = \frac{0.9\lambda}{\beta \cos\theta} \qquad (1)$$

where λ is the wavelength of CuKα target used (λ=1.5406 Å), β is full width at half maximum of the peak position in radian, θ is Bragg's diffraction angle at peak position in degree. The structural parameters such as crystallite size, strain and dislocation density are calculated for CuSe films are given in Table1. It is observed

from Table 1, that the value of crystallite size is found to increase, whereas the value of strain and dislocation density are found to decrease while increasing the deposition time from 20 to 40 minutes.

**Morphological and Optical Properties**

SEM image of CuSe thin films prepared at a deposition time of 40 minutes is shown in Fig.2. It is observed that number of crystallites are joined together to form grain which is shown in Fig.2. The non-uniform and undefined boundaries with different sizes are observed. The plot of (hv) versus $(\alpha hv)^2$ for CuSe thin films obtained at optimized condition is shown in Fig.3. Extrapolation of linear portion of the graph to the energy (hv) gives band gap energy of the material. The band gap value of the deposited film is found to be around 2.1 eV.

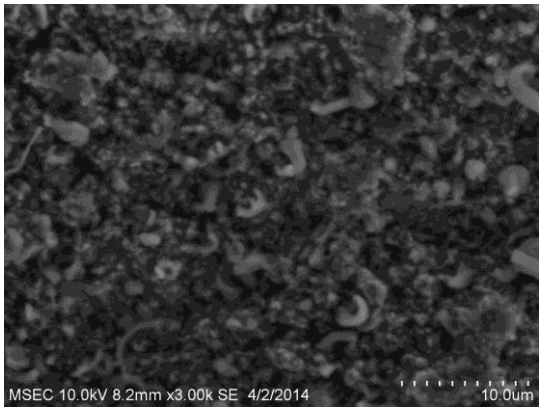


**Figure 2. SEM image of CuSe thin films prepared at a deposition time of 40 minutes.**

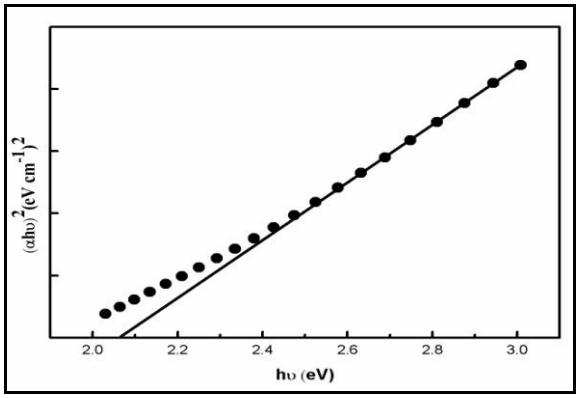


**Figure 3. Tauc's plot of CuSe thin films obtained at a deposition time of 40 minutes.**

## Conclusion

CuSe thin films were electrodeposited on ITO substrates. XRD patterns revealed that the deposited films were found to exhibit hexagonal structure with preferential orientation along (103) plane. Structural parameters were found to exhibit monotonic variation with deposition time and film thickness. Optical absorption analysis showed that the band gap value of the deposited film was found to be around 2.1 eV.

## Acknowledgement

One of the author (S.Thanikaikarasan) gratefully acknowledge the financial support received from the Board of Research in Nuclear Science Department of Atomic Energy (BRNS DAE), Mumbai, India with File No.2012/34/13/BRNS/No.166 to carry out this research work.

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