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Structural, Optical and Thermoelectric Properties of $Pb_{0.4}In_{0.6}Se$ Thin Films Deposited By Physical Evaporation Technique

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ABSTRACT

Thin films having different thickness of $Pb_{0.4}In_{0.6}Se$ were deposited by thermal evaporation techniques, onto precleaned amorphous glass substrate. The structural properties of films were evaluated by XRD, optical microscopy and EDAX. The optical properties of annealed thin films have been evaluated. The evaluated optical direct and indirect band gaps are 1.51 to 2.18 eV and 0.21 to 0.56 eV respectively. The X-ray diffraction analysis confirms that films are polycrystalline having orthorhombic structure. The average grain size is found to be 3.61 nm. Thermoelectric properties show a positive sign exhibiting P – type semiconducting nature of the film. The estimated values of Fermi energy and absorption coefficient are thickness dependent

Key words: optical microscopy, XRD, EDAX, optical properties, band gap, Fermi energy and absorption coefficient.

1. INTRODUCTION

In the recent years a fair amount of research has been carried out on PbSe and InSe because of their narrow band gap [1] and application in devices such as infrared devices [2,3], diodes [2,5], lasers, thermo photovoltaic conversions, solar cells [2-5], opto electronic devices, etc. Currently, electronic and optoelectronic industries provide some of the largest markets and challenges for thin film semiconductors. Current techniques for growth of these materials include physical methods. Physical methods are expensive but give relatively more reliable and reproducible results [6, 7]. InSe and PbSe based materials are of considerable technological interest for application to high speed and optoelectronic devices because of their high electron mobility and low effective electron mass [8-9]. The lead chalcogenides exhibit very interesting photoelectric, photoconducting, thermoelectric, optical and semiconductig properties [10]. Lead Selenide is important material of IV- VI group compounds. Due to its potential applications, thin films of lead chalcogenides have been extensively studied by doping N or P – type, so that they may be used in various solid state devices [11, 12]. From the study of literature review, it can be seen that no attempt has been made to study the variation of surface morphological study by change in thickness of thin films. In present work effect of film thickness on surface morphology over the thickness range 1000 – 3000 Å has been investigated. An attempt has been made to evaluate the optical band gap. Majority of these compounds have been reported to be grown in the crystalline form. Thin films preparation with direct materials do not shows any contamination of impurities, therefore the pure form of powder of Pb, In and Se was used for synthesis it.

2. EXPERIMENTAL

The compound ingot of $Pb_{0.4}In_{0.6}Se$ was obtained by mixing quantities of high-purity (99.999%) lead, indium and selenium powder in the atomic proportion 2:3:5. The mixture was sealed in an evacuated quartz tube at a pressure of 10^{-5} torr and heated at 1120 K for 36h and then quenched in ice cooled water. Polycrystalline $Pb_{0.4}In_{0.6}Se$ films have been deposited by physical evaporation technique under vacuum of about 10^{-5}torr. The substrate to source distance was kept 20cm. The samples of different thicknesses were deposited under similar conditions. The thickness of the films was controlled by quartz crystal thickness monitor model No. DTM-101 provided by Hind-HiVac. The deposition rate was maintained 5-10 Å/sec throughout sample preparation. Before evaporation, the glass substrates were cleaned thoroughly using concentrated chromic acid, detergent, isopropyl alcohol and distilled water.

X – Ray diffractogram (Rigaku Miniflex, Japan) were obtained of these samples to find out structural information and to identify the film structure qualitatively. The scanning angle (2θ) range was from 20^0 - 80^0 (CuK_α line). Optical absorption was measured by UV-VIS spectrophotometer model no. Shimadzu - 2450.The Thermoelectric power was measured by integral method [10] one end of the sample is heated while other end is held at constant temperature. The temperature difference between two ends of sample causes the emf generation. "Pushpa Scientific" Hyderabad provided the experimental set up used for the measurement of thermal emf. Maximum temperature gradient obtained was 150^0C in this set up.

3. Results and Discussion

3.1 Structural characterization

The structural composition of the grown films was studied through the optical microscopy, XRD analysis and EDAX.

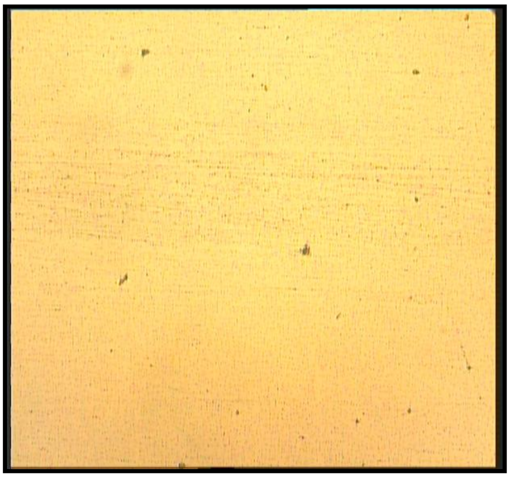

Fig. 1 Micrograph of $Pb_{0.4}In_{0.6}Se$ film of thickness 2000 Å

Fig. 1 shows the micrograph of $Pb_{0.4}In_{0.6}Se$ of thickness 2000 Å indicates particles are uniformly distributed over the surface. Further confirmation of the structure of the grown films was carried out using the x-ray diffraction pattern in Fig. 2.

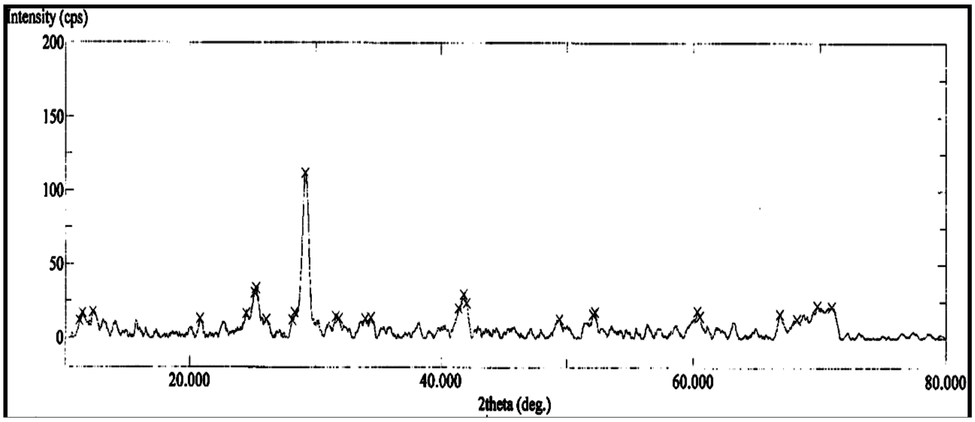

Fig. 2 XRD of $Pb_{0.4}In_{0.6}Se$ of thickness 1000 Å

Fig. 2 shows the XRD pattern of $Pb_{0.4}In_{0.6}Se$ thin film prepared at substrate temperature of 303k. The plane indices are obtained by comparing the intensities and position of the peaks with JCPDS data. There is no JCPDS slandered data available for different composition of $Pb_{1-x}In_xSe$. The presence of large number of peaks indicates that the films are polycrystalline in nature; exhibit the formation of the orthorhombic phase of $Pb_{0.4}In_{0.6}Se$. The unit cell volume is 768.23 and lattice parameters are a = 15.2960 Å, b = 12.3080 Å and c = 4.0806 Å. The value of the lattice parameters obtained from the analysis of x-ray diffraction pattern is as shown in Table 1. The structural parameters of $Pb_{0.4}In_{0.6}Se$ thin film shows that the film has average grain size of 3.61 nm for the film of thickness 1000 Å.

Table 1 Result obtained from X-ray diffractogram

Thickness Å	hkl	2θ degrees	D Å		FWHM rad	Grain Size nm	Average grain size nm
			Measured	Standard			
1000	200	11.40	7.7553	7.7553	0.003282	4.204	3.61
	030	20.82	4.2628	4.2628	0.004102	3.324	
	230	24.48	3.6332	3.6331	0.00288	4.704	
	201	25.16	3.5365	3.5365	0.002461	5.497	
	211	25.26	3.5227	3.5227	0.003701	3.655	
	301	28.14	3.1684	3.1684	0.004521	2.974	
	500	29.18	3.0578	3.0578	0.010683	1.255	
	321	31.64	2.8254	2.8254	0.003701	3.604	
	340	34.00	2.6345	2.6040	0.004521	2.932	
	700	41.40	2.1791	2.1791	0.003282	3.951	

The EDAX spectral analysis for the $Pb_{0.4}In_{0.6}Se$ thin film prepared by thermal evaporation technique is shown in Fig. 3. The obtained percentages of the constituent elements in all investigated films indicate that samples are nearly stoichiometric. The obtained results give support for the quality of the prepared

$Pb_{0.4}In_{0.6}Se$ thin films by thermal evaporation technique. The actual atomic % for $Pb_{0.4}In_{0.6}Se$ compositions of lead, indium and selenium are in the ratio of 19.90:29.31: 50.79.

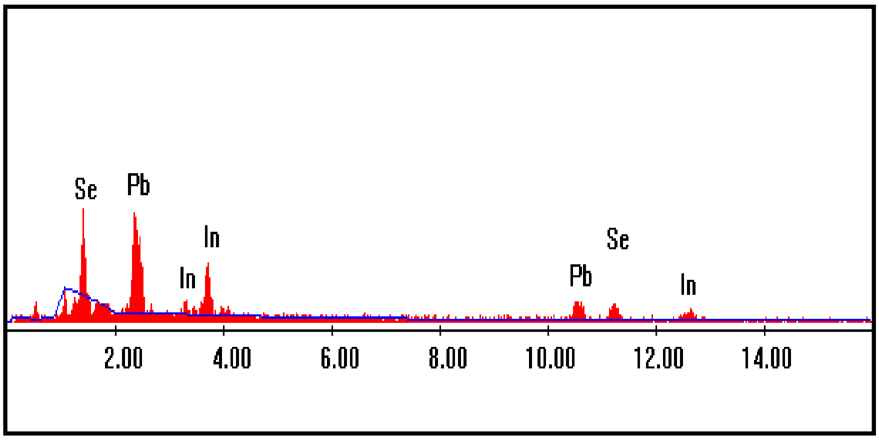

Fig. 3 EDS Spectra of $Pb_{0.4}In_{0.6}Se$ thin film

3.2 Optical properties of $Pb_{0.4}In_{0.6}Se$ thin films

The optical absorption spectra of $Pb_{0.4}In_{0.6}Se$ thin films for thickness 1000- 3000 Å was obtained in an UV-VIS –NIR spectrophotometer in the range 200- 1100nm. Figure 4 show the optical absorbance spectra of the films deposited in this work. The high absorbance in the UV region makes the material useful in forming p-n junction solar cells with other suitable thin film materials for photovoltaic applications. The optical band gap of these films has been calculated using the relation (Tauc 1974).

$\alpha h\nu = A(h\nu - Eg)^n$

And Extinction coefficient was calculated using the relation

Extinction coefficient = $\alpha\lambda/4\pi$

Where, $h\nu$ is the photon energy, α is the absorption coefficient, E_g the band gap, A is constant and, $n = 0.5$ for direct band gap material, $n = 2$ for indirect band gap material. Fig. 4 shows the plot of %T versus hυ. Fig. 5 shows the plot of α versus hυ and fig. 6 shows the plot of $(\alpha h\upsilon)^2$ versus hυ, from this graph the value of direct optical band gap was obtained by extrapolating these curves. Fig. 7 shows the plot of $(\alpha h\upsilon)^{1/2}$ versus hυ, from this graph the value of indirect optical band gap was obtained by extrapolating these curves. From fig. 5 the evaluated absorption coefficient and extinction coefficient are (0.5 - 3) x 10^5 [14] and (2.07- 13.3) x 10^{-3} respectively and from the fig. 6 and fig. 7 the evaluated optical direct and indirect band gaps are 1.51 to 2.18 eV and 0.21 to 0.56 eV respectively.

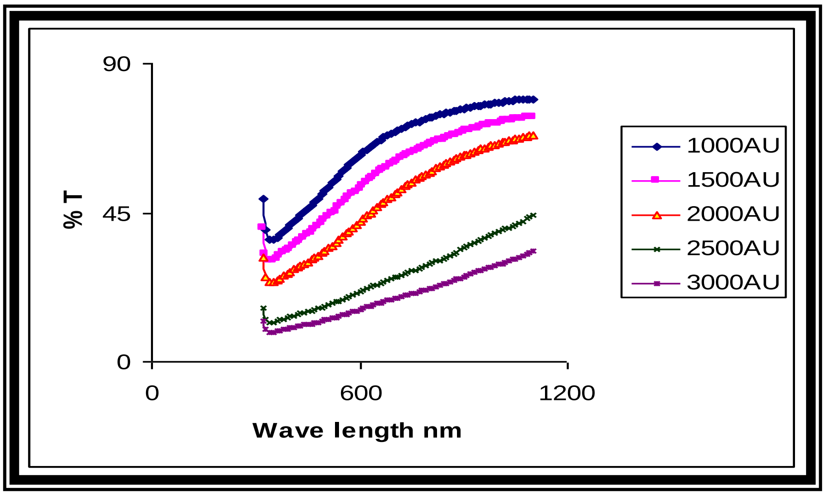

Fig 4 % T versus wavelength

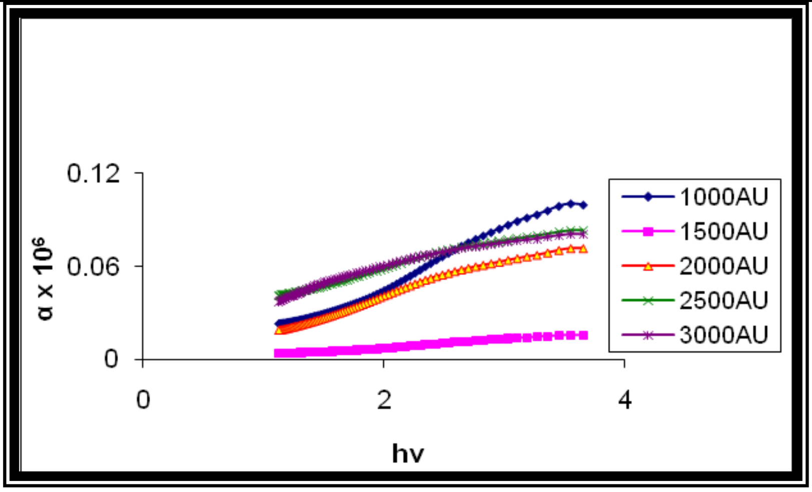

Fig 5 α x 10^6 versus hυ

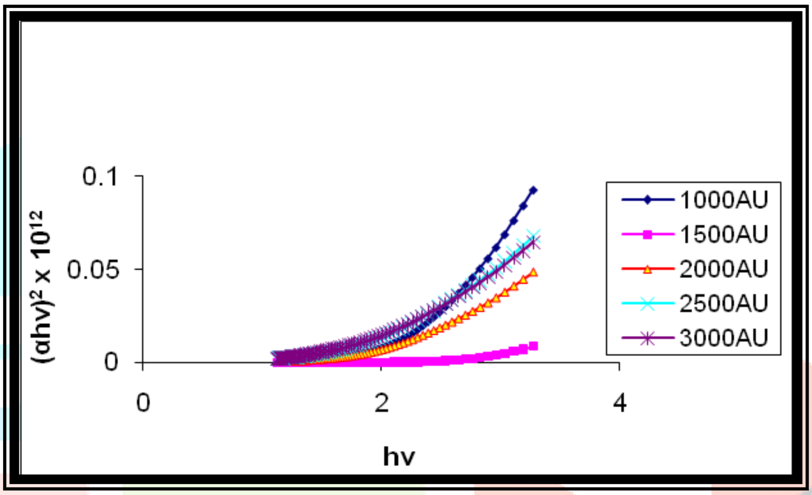

Fig 6 $(\alpha h\upsilon)^2$ versus hυ

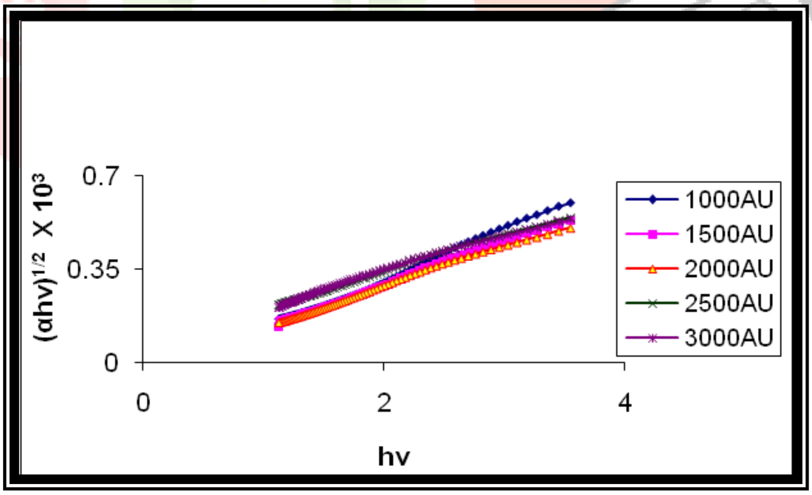

Fig 7 $(\alpha h\upsilon)^{1/2}$ versus hυ

3.3 Thermoelectric power measurement

The thermoelectric power (α) is measured by integral method [14, 15]. In integral method one end of the sample is heated while the other end is held at constant temperature. The temperature difference (ΔT) between two ends of sample causes the emf generation. "Pushpa Scientific" Hyderabad provided the experimental set up used for the measurement of thermal emf. Maximum temperature gradient obtainable is 150°C in this set up. The graphical representation of thermo emf versus change in temperature for different thickness of $Pb_{1-X}In_XSe$ (X=0.2) thin films are shown in Fig. 8 and the graphical representation of seebeck coefficient versus 1000/ΔT for different thickness is as shown in Fig 9 From this graph the Fermi energy and scattering parameter are calculated and represented in Table 2. The Fermi energy of $Pb_{1-X}In_XSe$ (X=0.2) thin films is thickness dependant. From TEP measurement, the deposited films are P- type semiconducting in nature [13-16].

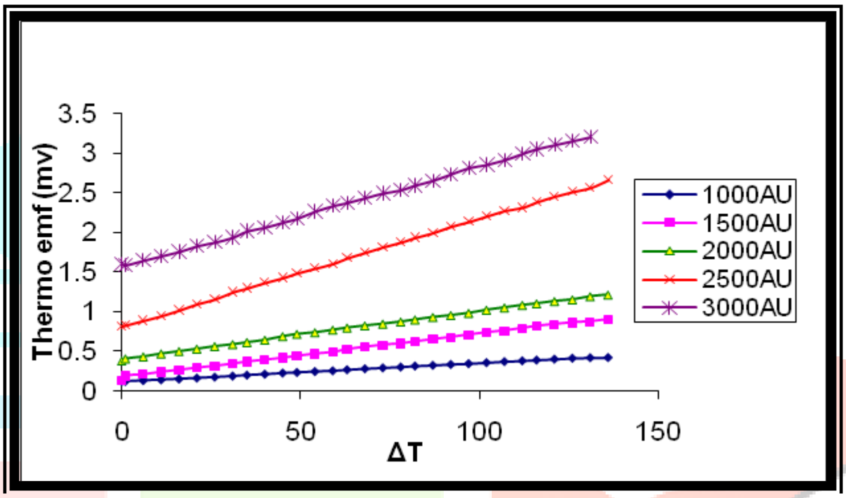

Figure 8 Thermo emf versus ΔT

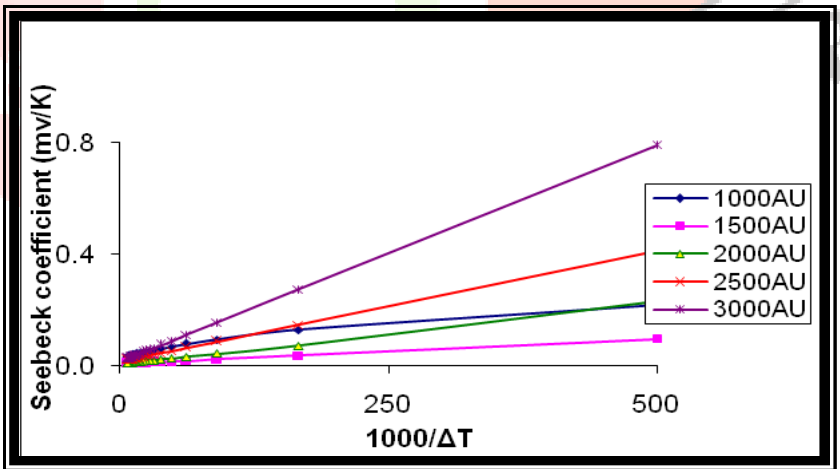

Figure 9 See beck coefficient versus 1000/ΔT

Table 2

Thickness Å	Fermi Energy (eV)	Scattering parameter
1000	0.02	0.26
1500	0.02	0.061
2000	0.04	0.07
2500	0.08	0.15
3000	0.16	0.143

4. Conclusion

The XRD shows that all the films prepared were polycrystalline orthorhombic structure. From the optical microscopy indicates particles are uniformly distributed over the surface. The evaluated absorption coefficient and extinction coefficient are (0.5 - 3) x 10^5 [14] and (2.07- 13.3) x 10^{-3} respectively. The optical direct and indirect band gaps are 1.51 to 2.18 eV and 0.21 to 0.56 eV respectively. From the temperature dependence of thermoelectric power, the Fermi energy E_f and scattering parameter increases with the thickness. The deposited films are P- type semiconducting in nature.

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