Structural and optical properties of $Pb_{0.8}In_{0.2}Se$ thin films

K. S. Chaudhari[1], Y. R. Toda[2], A. B. Jain[2], D. N. Gujarathi[2*]

[1]*S.V.S's Arts and Science College, Dondaicha*
[2]*Thin film laboratory, Department of Physics, Pratap College, Amalner(India)*

_____

ABSTRACT

$Pb_{0.8}In_{0.2}Se$ thin films were prepared on glass substrate by vacuum evaporation technique at a pressure of 10^{-5} torr. The structural properties of films were evaluated by XRD, EDAX, and optical microscopy. The x ray diffraction analysis confirms that deposited films are polycrystalline having cubic structure. The grain size was 54.11 to 56.73 nm. The optical properties of the films was determined over the thickness range of 2500Å and 3000 Å. Optical direct and indirect band gaps were calculated. The estimated direct and indirect optical band gaps were 0.816 to 0.85 eV and 1.71 to 1.78 eV.

Key words: XRD, EDAX, optical microscopy and Optical band gap.

_____

INTRODUCTION

Lead Selenide is important material of IV- VI group compounds. In the recent years a fair amount of research has been carried out on lead chalcogenides because of their application in devices such as infrared devices, diodes, lasers, thermo photovoltaic conversions, solar cells, opto electronic devices, etc (1-7). 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 (8). Majority of these compounds have been reported to be grown in the crystalline form. We have made an attempt to synthesize them in thin film form.

MATERIALS AND METHODS

The Indium doped PbSe alloy was prepared from its own constituent elements. Appropriate weight of lead, indium and selenium (purity 99.999%) were mixed together and placed in a quartz ampoule which was heated in furnace at temperature $1120^{0}C$ for 24 hours. Then cooled rapidly by ice cooled water. Thin films of $Pb_{0.8}In_{0.2}Se$ with varying thickness of 2500Å and 3000 Å were obtained on clean glass substrates held at room temperature, by vacuum evaporation technique at a pressure of 10^{-5} torr by thin film coating unit model no 12A4D. The lateral dimensions of the glass substrates of size 75mm $\times$ 25mm $\times$ 1.35mm were used and the source to substrate distance was kept as 20 cm. Quartz crystals monitor Model No. DTM 101,

was used to measure the thickness of the films. Films were deposited in the molybdenum boat at the evaporated rate 5 to10 A^0 per second. The deposition condition were maintained nearly the same during evaporation.

X–Ray diffractogram (Rigaku Miniflex, Japan) were obtained for finding out the structural information and qualitatively analysis of the grown films. The scanning angle (2θ) with the range of 20^0 - 80^0 (CuK$_\alpha$ line) was used for the XRD.

The optical absorption studies were carried out to estimate the band gap of the semiconductor films. The optical absorption spectra obtained in an UV-VIS-NIR spectrophotometer in the range 200 to 1100 nm at room temperature.

RESULTS AND DISCUSSION

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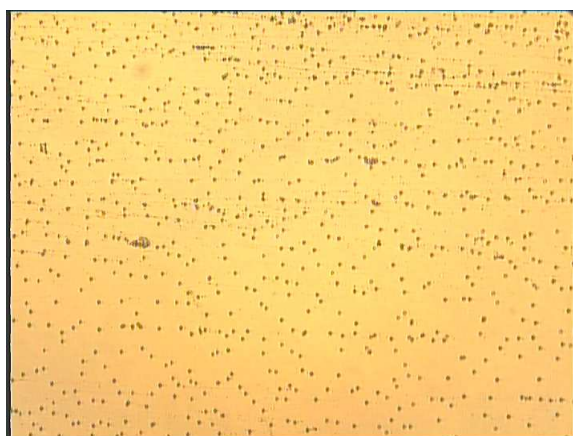

Figure 1 Micrograph of Pb$_{0.8}$In$_{0.2}$Se film of thickness 3000 Å

Fig. 1 shows the micrograph of Pb$_{0.8}$In$_{0.2}$Se of thickness 3000 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 Figure 2. The observed data have been compared with standard data, it is found that the deposited films are polycrystalline having cubic structure [6, 7]. The calculated values are as shown in table number 1.
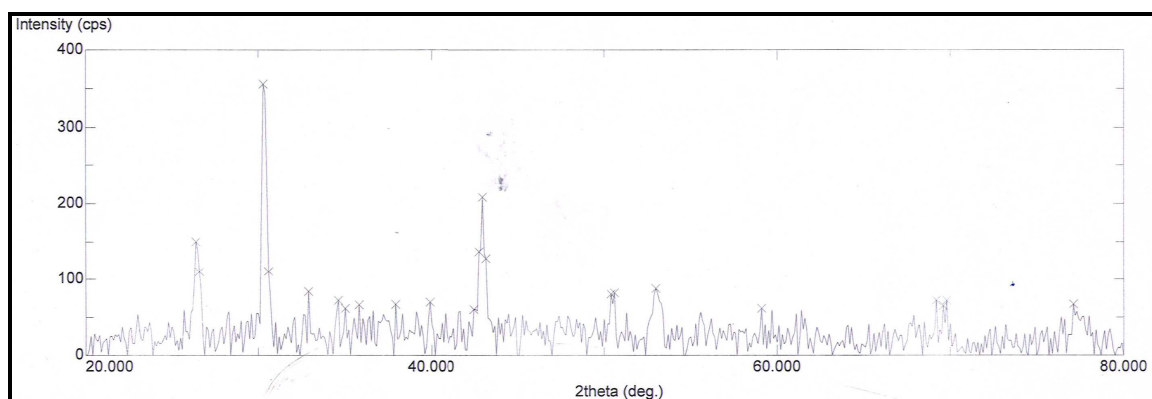

Figure 2 XRD of Pb$_{0.8}$In$_{0.2}$Se thickness 3000 Å

Table 1

Thickness Å	hkl	2θ Degree	D Å		FWHM rad	Grain Size nm	Average grain size nm
			Measured	Standard			
2500	---	30.20	2.9568	2.9568	0.00205	64.98	56.73
	311	30.40	2.9378	2.9378	0.00410	32.61	
	222	31.70	2.8202	2.8202	0.00205	64.74	
	320	32.50	2.7526	2.7526	0.00205	64.61	
3000	211	26.6	3.3482	3.3482	0.00205	65.50	54.11
	220	30.6	2.9190	2.9190	0.00205	64.92	
	300	32.9	2.7200	2.7202	0.00205	64.54	
	310	34.60	2.5902	2.5902	0.00616	21.48	
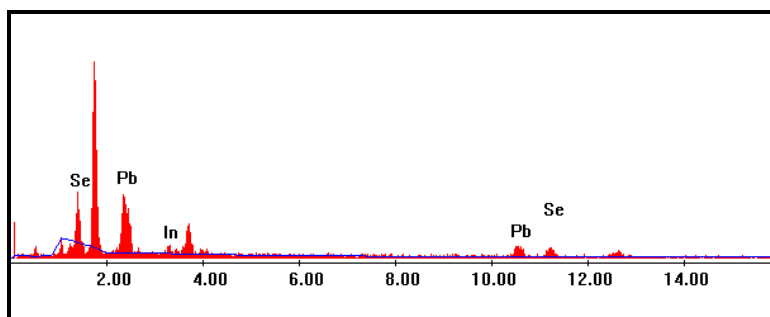
Figure 3 EDAX for $Pb_{0.8}In_{0.2}Se$ thin film

The stoichiometry and atomic wt % of $Pb_{0.8}In_{0.2}Se$ thin films was found by EDS. Figure 3 shows EDS spectrum of the as deposited $Pb_{0.8}In_{0.2}Se$ thin film. The actual atomic % for composition Lead, Indium and Selenium is found to be 37.26: 10.94: 51.80.

Optical properties

The optical absorption spectra were obtained in the 200nm-1100 nm wavelength range by employing a Shimadzu 2450 UV-Visible model of the spectrophotometer. Figure 4 shows the optical absorbance spectra verses wave length range nm of the films deposited in this work. To find α, the relation used is given by $\alpha = -1/d \ln T$, where T is the transmittance and d is the thickness of the film at room temperature.

The fundamental absorption edge is one of the most important features of the absorption spectrum of a semiconductor. The increased absorption near the edge is caused by the transition of electron from the valance band to conduction band. Figure 5 shows the plot of absorption coefficient α against photon energy. The value of fundamental absorption edge from the intercept lies at 1.13-1.16 eV and the corresponding α values were 0.12×10^6 to 0.5×10^6 cm^{-1}. The higher value of α in the UV region makes the material useful in forming p-n junction, solar cells with other suitable thin film materials for photovoltaic applications [14].

The optical band gap of these films has been calculated using the relation (Tauc 1974).

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

Where, $h\nu$ is the photon energy, α is the absorption coefficient, Eg the band gap, A is constant and, $n = 0.5$ for direct band gap material, $n = 2$ for indirect band gap material. Figure 6 shows $(\alpha h\nu)^{1/2}$ verses photon energy for $Pb_{0.8}In_{0.2}Se$ thin films which shows the value of direct optical band gap for films. Figure 7 shows $(\alpha h\nu)^2$ verses photon energy for $Pb_{0.8}In_{0.2}Se$ thin films

which shows the value of indirect optical band gap for films.   The direct and indirect energy band gaps of these samples were 0.816 to 0.85 eV (12) and 1.71 to 1.78 eV (10, 11, 12) respectively.
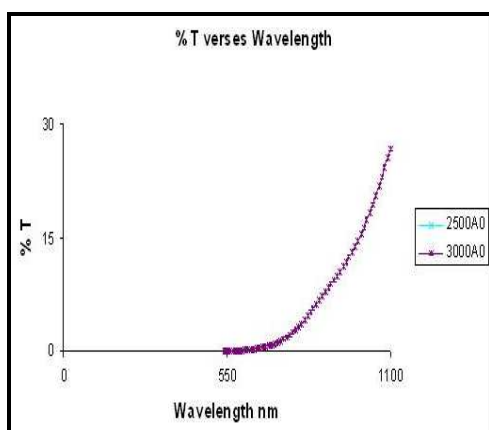

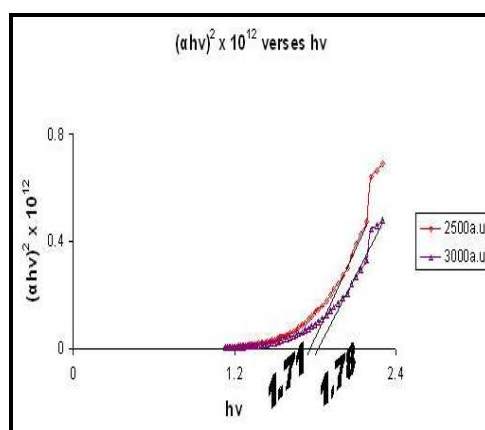**Figure 4   Plot of % T verses Wave length nm.**
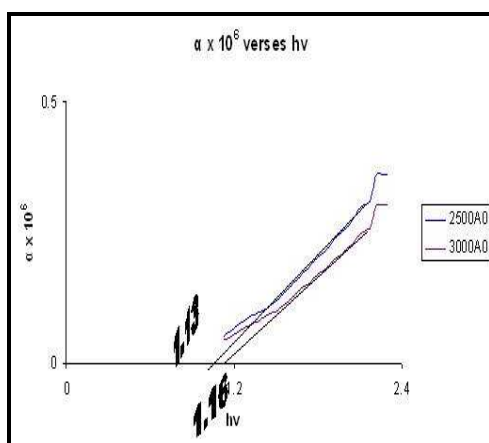

Fig 6 $(\alpha h\nu)^2$ x 10^{12} Vs hν

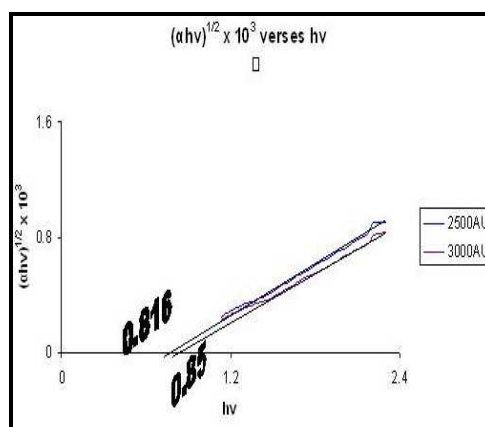**Figure 5 Plot of α x 10^6 verses *h*ν**

Fig 7 $(\alpha h\nu)^{1/2}$ x 10^3 Vs hν

CONCLUSION

- ✓ Thin films of $Pb_{0.8}In_{0.2}Se$ were deposited successfully.
- ✓ From XRD the deposited samples are polycrystalline having cubic structure and grain size was 54.11 to 56.73 nm.
- ✓ The estimated direct optical band gap   was 0.816 to 0.85 eV.
- ✓ The estimated indirect optical band gap   was 1.71 to 1.78 eV.
- ✓ Optical analysis revealed that prepared $Pb_{0.8}In_{0.2}Se$ thin films were direct allowed and it is suitable absorber layer for photovoltaic application.

REFERENCES

[1] Y.Badr and M.A. Mohmoud, *Cryst. Res. Technol*, **2006,** 41 (7), 658.

[2] Matt low, Joseph M. Luther, Qing Song, Barbata , K. Hughes*, J. of Chem Soc*, **2008,**130, 5974.

[3] Zhen Li, Chao Wu, Yanyan Liu,Tiebing Liu, Zheng Jiao and Minghong Wu, *Bul of Mater Sci,* **2008**, 31(6), 825.

[4] S. Prabahar, N. Suryanarayanan, K. Rajasekar, S.Srikanth, *Chal. Letters*, **2009,** 6 (5), 203.

[5] S. Prabahar,   N. Suryanarayanan, S. Srikanth,   S. Srikanth, D. Kathirvel, *Chal. Letters*, **2009, 6** (9)**,** 203.

[6] K R Murali, P Ramanathan, *Chalcog.   Letters* **2009**, 6 (3), 91.

[7] Chaya   H. Ben - Porat, Oksana Cherniarskaya,   *J. Phys. Chem. A*, **2004,** 108, 7814.

[8] S. P. Sing, S. Kumar, *J. Of Mater. Sci*, **2005**, 40, 481.

[9] H.K. Sachar, I Chao, P.J.McCann and X. M.Fang, *J. of Appl. Phys*., **1999,** 85 (10), 7398.

[10] Wenjie Lcang, OdedRabin, Allon Hochbaum,Melissa Fardy,Minjuan Zhang, *Nano Re*s, **2009**, 2, 394.

[11] Hui Du, Chialing Chen, Rishikesh Krishnan, Todd D. Krauss, *Nano Letters*, **2002**, 2 (11), 1321.

[12] A. K. Pattanaik, A.Srinivasan, *J.of Optoelectronics and Adv. Materials*, **2003**, 5(5), 1161.

[13] D. Kumar and S. Kumar, *Bull. Mater. Sci*, **2004**, 27(5), 441.

[14] B. Kavitha, M. Dhanan, *J. Of Ovonic   Res*, **2010,** 6(2), 75.

[15] S. N. Sahu, *Thin solid films*, **1995,** 26, 98.