

LEAD SELENIDE THIN FILMS FROM VACUUM EVAPORATION METHOD-STRUCTURAL AND OPTICAL PROPERTIES

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Thin films of PbSe of different thickness have been prepared on glass substrates in room temperature by vacuum deposition. The thickness of the deposited films is measured by employing quartz crystal monitor method. PbSe thin film of thickness 500 Å has amorphous structure. When the increase in thickness is from 1000 Å to 2000 Å, the films have polycrystalline structure which are identified by X-ray diffraction, scanning electron microscopic and atomic force microscopic studies. The structural parameters such as interplanar distance (d), lattice parameter (a), grain size (D), dislocation density (ρ) and microstrain (ϵ) have been evaluated. The optical properties have been studied in the range of wavelength 2500-5000nm. The optical band gap values of different thicknesses have been estimated and reported in this paper.

(Received April 29, 2009; accepted May 3, 2009)

Keywords: Structural properties, X-ray diffraction, Scanning electron microscopy, Atomic force microscopy, Vacuum deposition, Optical Properties

1. Introduction

Lead chalcogenides (PbSe, PbTe, PbS) are important materials for applications such as IR detectors, photographic plates, and photo resisters [1-3]. Among the group IV-VI compounds, Lead selenide (PbSe) thin film is used as a target material in infrared sensor, grating, lenses and various opto electronic devices [4]. It has a cubic crystal structure (higher thickness) and a direct band gap of 0.27 eV in room temperature. This paper deals with the structural, surface analysis and optical studies of PbSe thin films prepared from thermal vacuum evaporation technique.

2. Experimental

Lead selenide thin films are prepared by thermal vacuum evaporation technique onto glass substrate, at vacuum of 10^{-6} Torr. Lead selenide powder (Merk) is used with the purity of 99.99%. The experimental arrangement is permitted to prepare thin films samples under various conditions. The thicknesses of the films ranging 500, 1000 and 2000 Å are measured by a quartz crystal monitor method. The structural analysis of films is performed by X-ray diffractometer (Bruker AXS D8). The surface morphology of the films is investigated by means of atomic force

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microscopy (AFM) and scanning electron microscopy (SEM). The transmission and absorption spectra are recorded using FTIR spectrophotometer (Model NEXUS 670) in the range of 2500-5000nm, at room temperature.

3. Results and discussion

3.1 Structural analysis of PbSe thin films

X-ray diffractogram of PbSe thin films, taken from diffractometer is used to analyze various crystalline aspects. According to the Bragg's law,

$$n\lambda = 2d_{hkl}\sin\theta_{hkl} \quad (1)$$

the direction of propagation of scattered beams (θ_{hkl}) is related to the inter planar distance (d_{hkl}) in the lattice hkl which represents the property of the material and is related with the lattice constant and miller indices [5]. The XRD pattern for PbSe thin films of thickness 500Å, 1000Å and 2000 Å are shown in Fig. 1, Fig. 2 and Fig. 3.

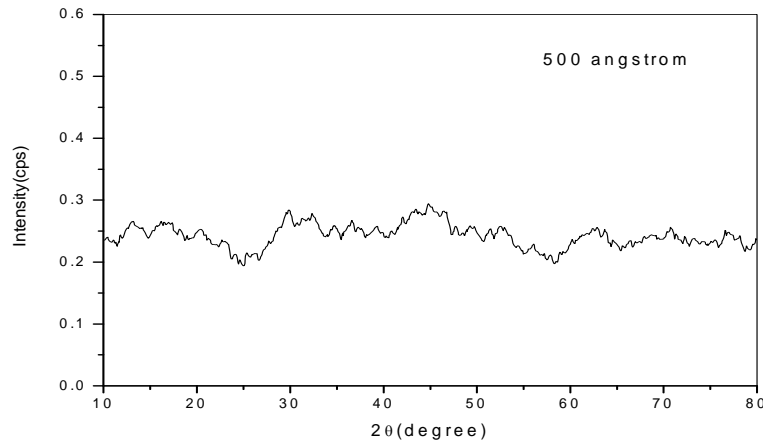


Fig. 1. X-ray diffractogram of PbSe thin film of thickness 500 Å

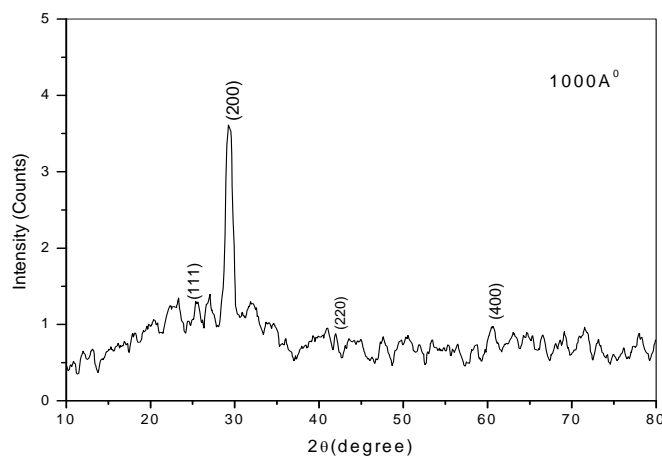


Fig. 2. X-ray diffractogram of PbSe thin film of thickness 1000 Å

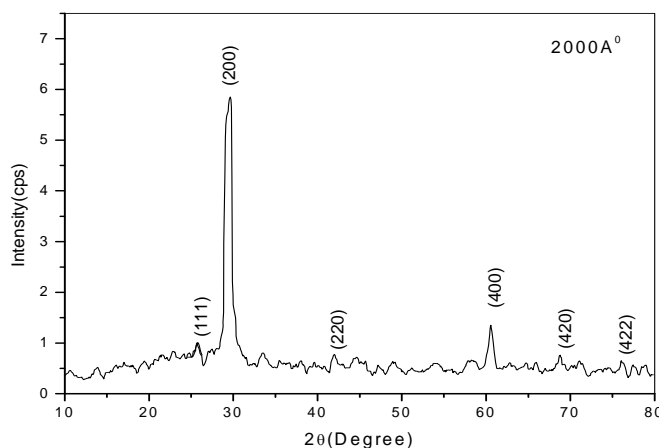


Fig. 3. X-ray diffractogram of PbSe thin film of thickness 2000 Å

Fig. 1 shows that the PbSe thin film of thickness 500 Å has no particular distinctive and prominent peaks, which confirm the amorphous nature of the evaporated material. In the case of films with higher thickness, 1000 Å and 2000 Å, there is a prominent peak in 2θ values which correspond to (200) plane and the other peaks at different 2θ values observed are weak which are shown in Fig. 2 and 3. The presence of large number of peaks indicates that the film is polycrystalline in nature [6].

The predominant growth of crystallites perpendicular to (200) plane, gives rise to the rock salt cubic structure of PbSe as indicated in the ASTM [1, 7, 8]. The intensity and number of peaks are observed to be greater in film having thickness 2000 Å, when compared to those of film thickness 1000 Å. This fact indicates that the degree of crystallinity is found to be more pronouncing in films of higher thickness. The inter planar distance (d) and the lattice parameter (a) are calculated in this case by means of the plane-spacing equation for cubic crystal, which is given by,

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \quad (2)$$

and the grain size is calculated by using the Scherer's formula,

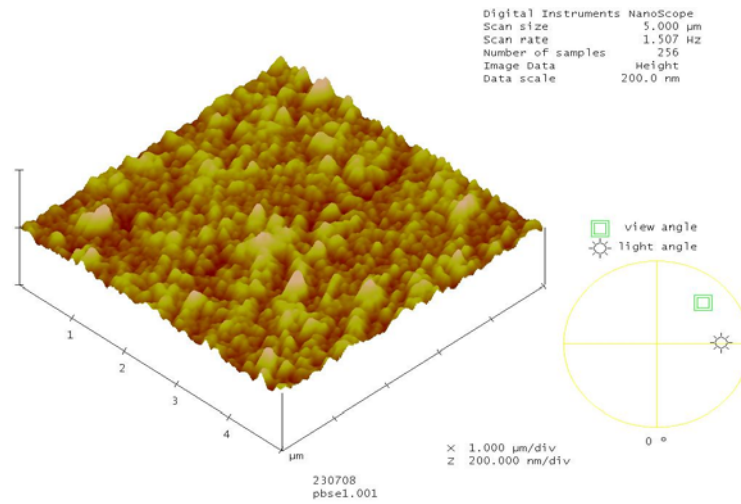
$$D = \frac{k\lambda}{\beta \cos \theta} \quad (3)$$

The interplanar distance (d), lattice parameter (a), grain size (D), dislocation density (ρ) and microstrain (ϵ) are given in the Table 1.

Table 1. Structural parameters of PbSe thin films

Thickness \AA	hkl	$d(\text{\AA})$ Exp	$d(\text{\AA})$ $ASTM$	2θ	$A(\text{\AA})$	$FWHM$ (β)	Grain Size(D) \AA	Dislocation Density (δ) 10^{15} $lines/m^2$	Strain(ϵ) 10^{-3}
1000	111	3.4883	35340	25.5141	6.0419	0.56080	151.7875	4.3405	9.5408
	200	3.399	3.0606	29.3570	6.0798	0.4168	208.5879	2.3593	7.0341
	220	2.1502	2.1642	41.9846	6.0817	0.2578	344.9752	0.8403	4.1978
	400	1.5274	1.5303	60.5693	6.1098	0.7425	129.4681	5.9658	11.1854
2000	111	3.4882	3.5340	25.5155	6.0418	0.1074	792.5242	0.1592	1.8273
	200	3.333	3.0606	29.4218	6.0667	0.2383	843.988	0.1404	4.1569
	220	2.1543	2.1642	41.9013	6.0933	0.2344	379.2831	0.6951	3.8182
	400	1.5275	1.5303	60.5697	6.1098	0.4035	238.2303	1.7619	6.0788
	420	1.3629	1.3687	68.8299	6.0950	0.5038	199.7445	2.5064	7.2500
	422	1.2477	1.2494	76.2470	6.1126	0.2378	443.8548	0.5076	3.2627

From the Table-I it is found that, the grain size of the film increases with film thickness and the dislocation density and micro strain are found to decrease. It can be attributed to the decrease in the imperfections and dislocations of the films with increasing film thickness. It is also observed that FWHM decreases with thickness. This decrease in the value of FWHM indicates a residual increase in crystalline size or a decrease in residual micro-strain.

Fig. 4. AFM micrographs of PbSe thin film of thickness 500 \AA

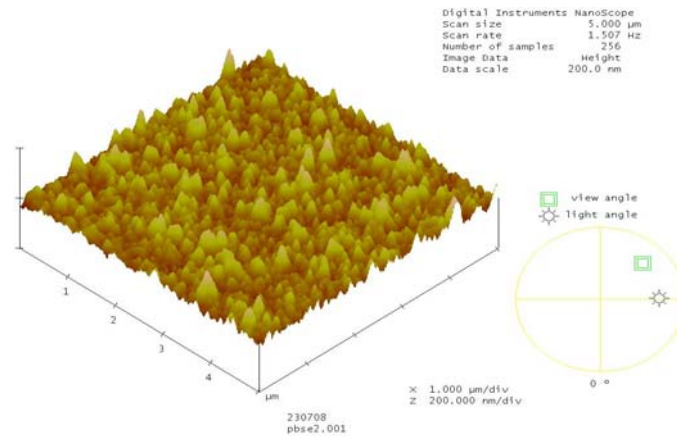


Fig. 5. AFM micrographs of PbSe thin film of thickness 1000 Å

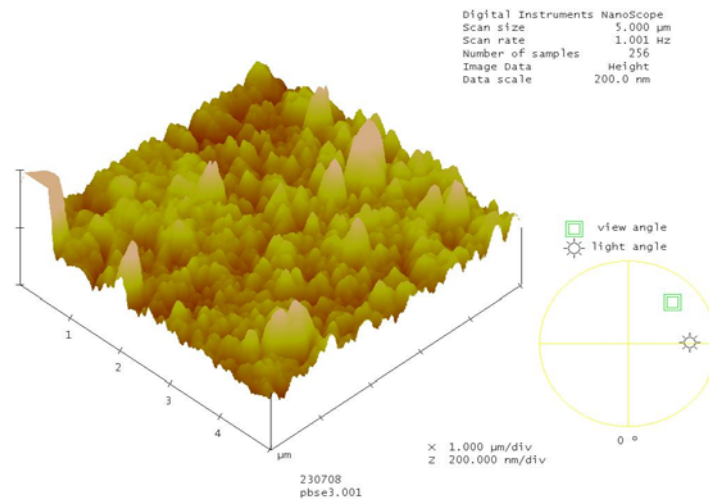


Fig. 6. AFM micrographs of PbSe thin film of thickness 2000 Å

Fig. 4, Fig. 5 and Fig. 6, show the three-dimensional view of AFM micrographs of lead selenide thin films having thickness of 500 Å, 1000 Å and 2000 Å respectively. The scanning is done over an area of $5\mu\text{m} \times 5\mu\text{m}$. The micrographs show that the surfaces of the lead selenide thin films which consist of nanoscale particles are dense. The maximum size of particles and the roughness of the surface of PbSe films of thickness 500 Å, 1000 Å and 2000 Å are tabulated in Table-II

Table 2. Variation of particle size with thickness

Film thickness (Å)	Particle size (nm)	Roughness of the surface (nm)
500	68	10.12
1000	94	15.80
2000	151	22.00

The increase film thickness corresponds to the particle size increase in the AFM study which well matches with the results obtained from XRD.

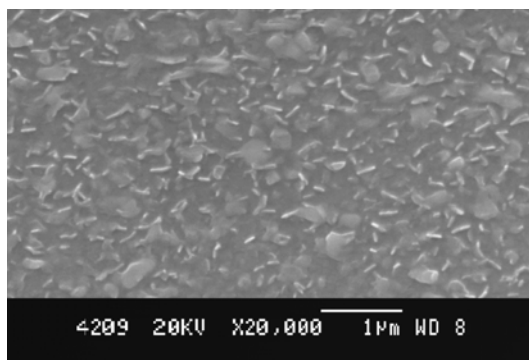


Fig. 7. Scanning electron micrographs of PbSe thin film of thickness 500 Å

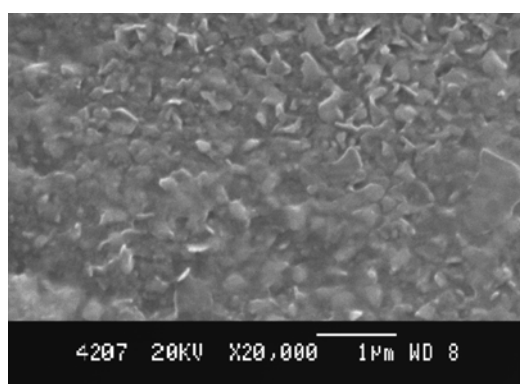


Fig. 8. Scanning electron micrographs of PbSe thin film of thickness 1000 Å

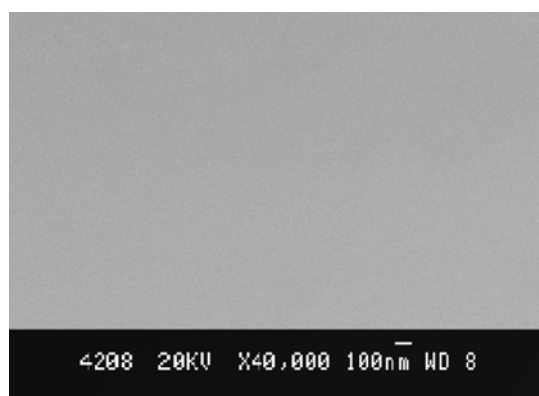


Fig. 9. Scanning electron micrographs of PbSe thin film of thickness 2000 Å

Fig. 7, Fig. 8 and Fig. 9 show the SEM images of lead selenide thin films of different thicknesses. The SEM micrograph of thickness 500 Å is analyzed at a resolution of 1µm with 20,000X magnification. Mosaic structure along with irregular shaped grains is observed that are uniformly distributed over the surface which is represented in Fig. 7.

The grains are found to be thickly packed, and inter grain spacing is reduced in the case of film thickness 1000 Å as shown in Fig. 8. This results in film with better crystallinity. The SEM micrograph taken for film of higher thickness at a resolution of 100nm and with 40,000X magnification indicates a smooth and homogeneous surface shown in Fig. 9. This may be due to the high-preferred orientation of the film in the (200) plane.

3.2 Optical Properties

Optical transmittance and absorption spectra of PbSe thin films which are measured as a function of the wavelength of incident photons of different thickness are shown in Fig. 10 and 11.

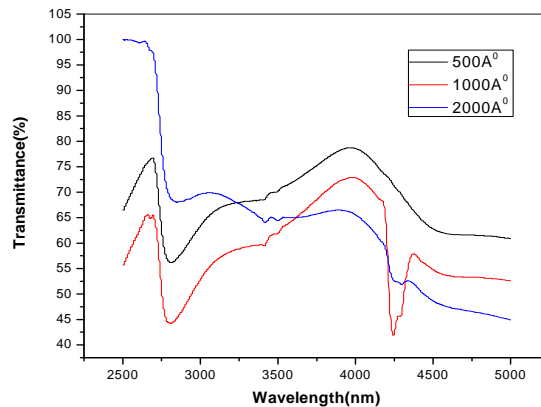


Fig. 10. Transmittance spectra of PbSe films for various thicknesses.

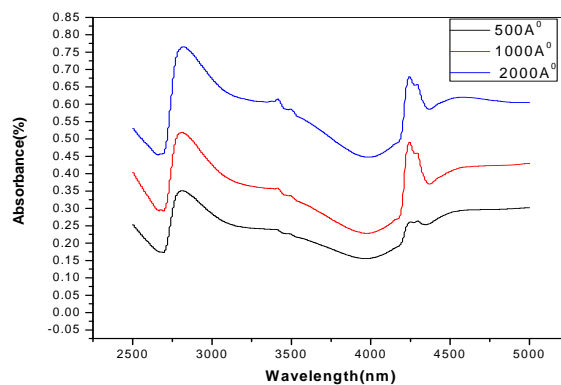


Fig. 11. Absorbance spectra of PbSe thin films for various thicknesses

Fig. 10 indicates a decrease in the transmittance with increase in film thickness, which leads to a decrease in light scattering losses [9]. The absorbance is observed to be increasing with increase in film thickness which is revealed in Fig. 11. It can be concluded that the absorbing nature in material is high.

Variation of extinction coefficient (K_f) with wavelength is as shown in Fig. 12.

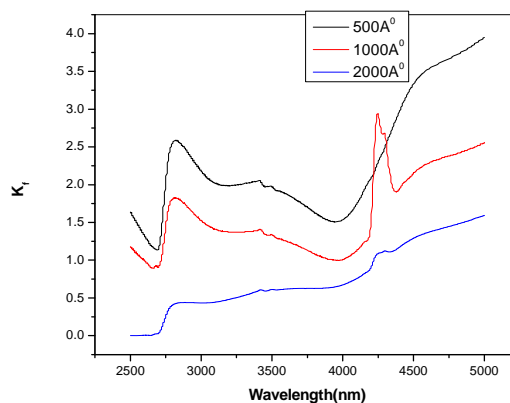


Fig. 12. Thickness dependence of extinction coefficient (K_f).

From the Fig.12 that the value of extinction coefficient (K_f) decreases with increase in film thickness, which may be due to the improvement of the crystallinity, whereas the increase in film thickness leads to the minimum imperfections. A plot of $(\alpha h\nu)^2$ Vs $h\nu$ of PbSe thin films having various thicknesses is given in Fig. 13,14 & 15.

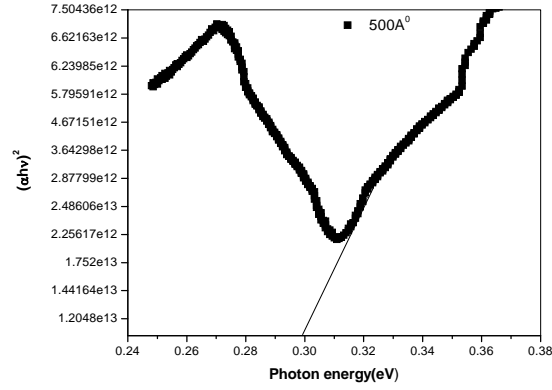


Fig. 13. A Plot of $(\alpha h\nu)^2$ Vs. $(h\nu)$ for PbSe thin film of thickness 500 Å

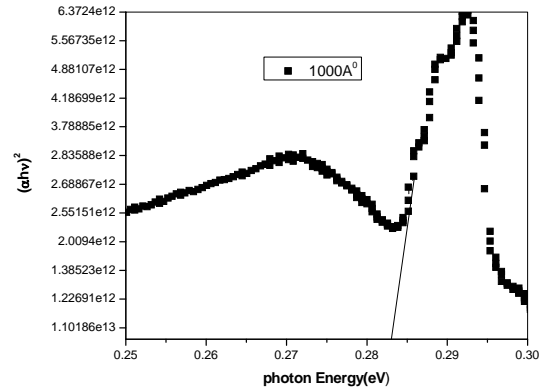


Fig. 14. A Plot of $(\alpha h\nu)^2$ Vs. $(h\nu)$ for PbSe thin film of thickness 1000 Å

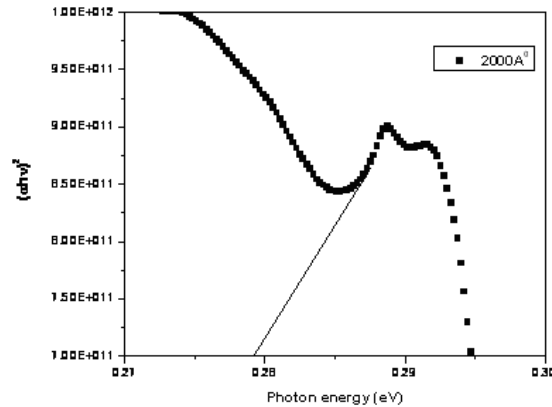


Fig. 15. A Plot of $(\alpha h\nu)^2$ Vs. $(h\nu)$ for PbSe thin film of thickness 2000 Å.

The energy gaps for these films are obtained by extrapolating the linear straight line portion of the curve to the energy axis. The variation of energy gap with thickness is shown in the Table-III.

Table 3. Variation of energy gap with thickness

Film thickness	Bandgap energy (E_g) eV
500 Å	0.299
1000 Å	0.283
2000 Å	0.279

From the Fig. 13, 14 and 15 it is observed that PbSe thin film exhibits direct band transition and its band gap energy decreases with increase in film thickness. Hence the variations of band gap in the films are due to the changes in the lattice constant.

5. Conclusions

From the present study it can be concluded that the PbSe thin films is prepared in three different thicknesses. The amorphous nature is formed when the thickness is in 500 Å. When thickness is in higher level (i.e. 1000 Å and 2000 Å) the polycrystalline structure is observed by X-ray diffraction analysis. Further, the surface morphological studies show that the sizes of the particles increase along with thickness of the film by the means of AFM. By using FTIR spectrophotometer, the transmittance and absorbance spectra in the range of 2500-5000 nm have been taken. In absorbance spectra, the material has a high absorbing nature. The observed band gap energy is inversely dependent on film thickness.

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