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Optical and AFM studies on Lead Selenide thin films

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ABSTRACT

Thin films of PbSe of different thicknesses have been prepared on glass substrates at room temperature by vacuum deposition. The thickness of the deposited films was measured by employing quartz crystal monitor method. The optical properties have been studied in the range of wavelength 2500-5000nm.The optical band gap, absorption coefficient extinction coefficient values of different thicknesses have been estimated and reported in this paper. The surface morphology of the films is investigated by means of atomic force microscopy (AFM).

Keywords: Optical Properties, Atomic force microscopy, Vacuum deposition.

INTRODUCTION

The small energy gap of lead chalcogenide semiconductors is one of the most important properties leading to the great experimental interest in these materials [1].Owing to their narrow band gap PbSe have been used in infrared applications for decades. PbSe is classified as a narrow band gap semiconductor with E_g=0.29eV and widely employed to produce Photo resistors, Photo detectors and Photo emitters in the IR range as well as Injection lasers[2].These materials can be obtained in thin film form by various methods including vacuum deposition [3], chemical bath deposition[4],electro deposition[5], Sono chemistry [6] and microwave heating[7].The vacuum deposition method is relatively inexpensive, simple and convenient for the large area deposition of IV-VI compounds. Hankare etal [1] have studied structural, optical and electrical properties of PbSe this films prepared by Chemical bath deposition method. They have also reported XRD study confirms Poly crystalline nature in FCC structure. The optical absorption spectrum showed an exponential edge. Room temperature electrical conductivity was the order of 10^{-3} ohmcm^{-1}. The film exhibits p-type conductivity. Sushil kumar etal [3] have

prepared PbSe thin films by vacuum deposition and studied their optical, structural and electrical properties. The values of absorption co-efficient, band gap, conductivity and activation energy reported are $.78\times10^{4}$, 0.29eV, 5.51×10^{-2} and 0.14 respectively. Photoconductivity measurements have been performed by Roberts etal [8] on PbSe thin films prepared by chemical bath deposition method. Robert et al also reported that no evidence is found to support the theory of barrier- modulated photoconductivity but rather one of barrier inhibited conductivity. The present work deals with the optical and AFM analysis of PbSe thin films prepared by thermal evaporation.

MATERIALS AND METHODS

High purity PbSe (99.999% Aldrich company,USA) thin films of different thicknesses (500Å,1000Åand 2000Å)are prepared onto glass substrates kept at room temperature by thermal evaporation using HINDHIVAC 12 vacuum coating unit under a 10^{-6} torr. A molybdenum boat is used as the evaporation source and the substrates are placed directly above the source at a distance of nearly 25cm.The glass substrates are freshly cleaned with detergent solution and distilled water followed by ultrasonic agitation. The rate of deposition and thickness of the films are measured and controlled *in situ* HIND-HIVAC quartz crystal thickness monitor. The rates of deposition are maintained ~1Å/s. The transmission and absorption spectra is recorded using FTIR spectrophotometer (Model NEXUS 670) in the range 2500-5000nm, at room temperature. The surface morphology of the films is investigated by means of atomic force microscopy (AFM).

RESULTS AND DISCUSSION

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. 1 and 2.

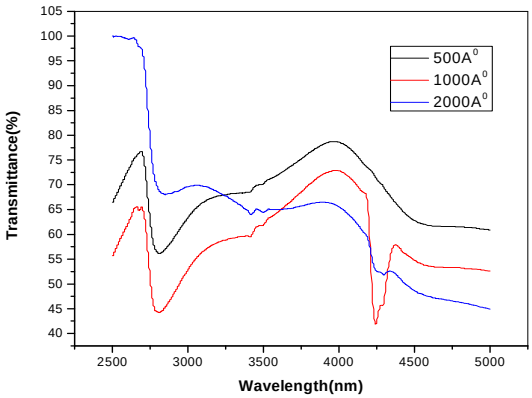

Fig.1. Transmittance spectra of PbSe films for various thicknesses

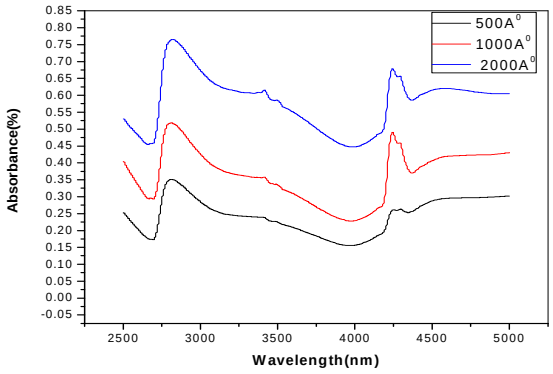

Fig.2. Absorbance spectra of PbSe thin films for various thicknesses

Fig.1 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. 2. 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. 3.

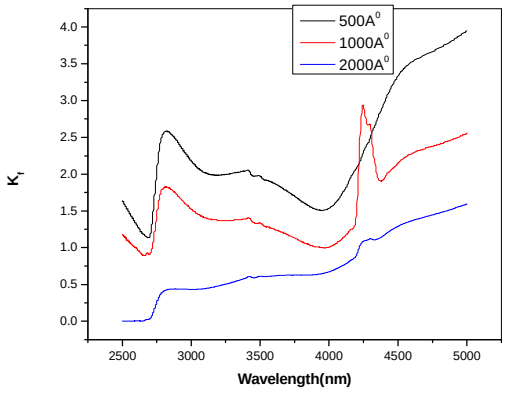

Fig. 3. Thickness dependence of extinction coefficient (K_f)

From the Fig.3 that the value of extinction coefficient (K_f) decreases with increase in film thickness, which may be due to the improvement of the crystallanity.Whereas the increase in film thickness leads to the minimum imperfections. A plot of $(\alpha h\nu)^2$ Vs hν of PbSe thin films having various thicknesses are given in Fig. 4,5and 6. The absorption coefficient of PbSe thin films with different thickness was calculated using the transmittance (T) value measured for a particular wavelength and thickness (t) using the relation

$$\alpha = -\ln (T)/t \text{----------1}$$

The extinction coefficient is calculated using the relation

$$K = \alpha\lambda/4\pi \text{ ----------2}$$

The absorption coefficient can be said to be governed by the Urbach relation

$$\alpha = A (h\nu - Eg)^p / h\nu \text{----------3}$$

Where A is a constant, E_g is the energy gap, is the frequency of the incident radiation and h is Planck's constant. The exponent p is 0.5 for direct allowed transitions, 2.0, for indirect allowed transitions, and p is 3.0 for indirect forbidden transitions. Fig 4, 5 and 6 shows the plot $(\alpha h \nu)^2$

vs. hν, i.e. with p=0.5 for PbSe thin film of thickness 500 Å ,1000 Å and 2000 Å. The presence of a single slope in the curves suggests that films from thermal evaporation are of single phase in nature and the type of transition is direct and allowed [3]. At higher wavelengths the non-linear tail absorption in the curves may be due to transitions associated with the absorption of longer wavelength phonons as reported earlier [10]**.** The energy gaps of the films of various thicknesses have been determined by extrapolating the linear portion of the plots of $(\alpha h\nu)^2$ against hν to the energy axis. The calculated band gaps of the films are in good agreement with the reported values **[**3**]**. The lowering of the band gap may be due to the presence of impurity electronic levels in the forbidden gap We do not observe a straight-line behaviors on graphs of $(\alpha h\nu)^{2/3}$ vs. hν (direct forbidden), $(\alpha h\nu)^{1/2}$ vs. hν (indirect allowed) $(\alpha h\nu)^{1/3}$ vs. hν (indirect forbidden). These plots (not shown) reveal that the type of transition is neither direct forbidden nor indirect.

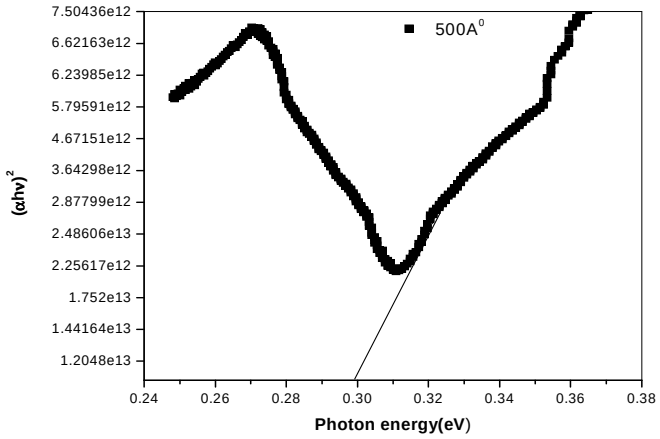

Fig.4. A Plot of $(\alpha h\nu)^2$ Vs. (hν) for PbSe thin film of thickness 500 Å

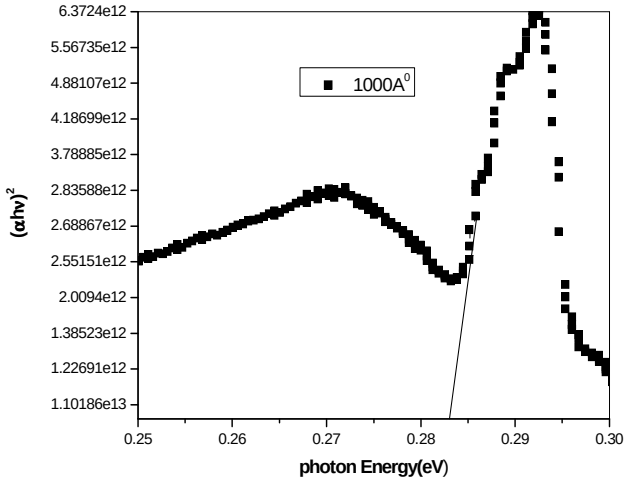

Fig. 5. A Plot of $(\alpha h\nu)^2$ Vs. (hν) for PbSe thin film of thickness 1000 Å

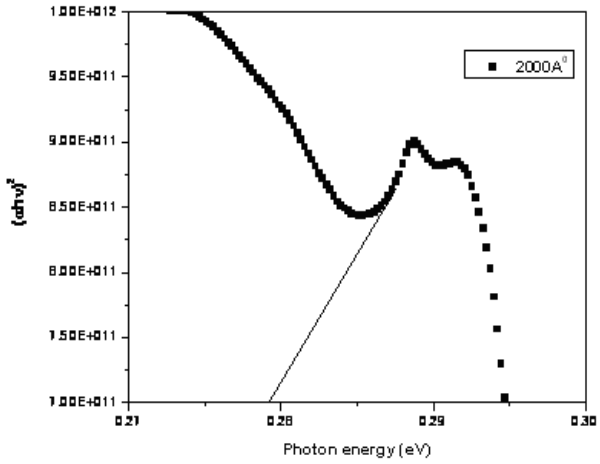

Fig.6. A Plot of $(\alpha h\nu)^2$ Vs. (hν) for PbSe thin film of thickness 2000 Å.

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, Extrinsic coefficient and absorption coefficient with thickness is shown in the Table-I.

Table 1. Variation of Energy gap, Extrinsic Coefficient and Absorption Coefficient with thickness

Film thickness	Bandgap energy (E_g) eV	Extrinsic coefficient	Absorption coefficient
500 Å	0.299	5.18	1.35
1000 Å	0.283	4.85	1.37
2000 Å	0.279	4.59	1.41

From the Fig. 4, 5 & 6 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.

AFM ANALYSIS

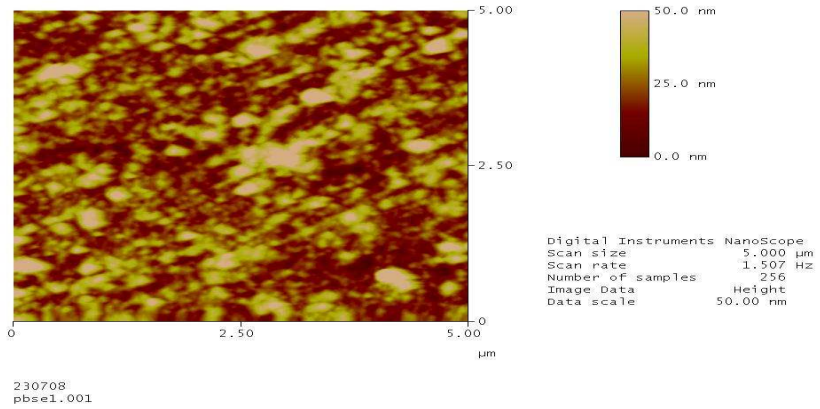

Fig.7. AFM micrographs of PbSe thin film of thickness 500 Å

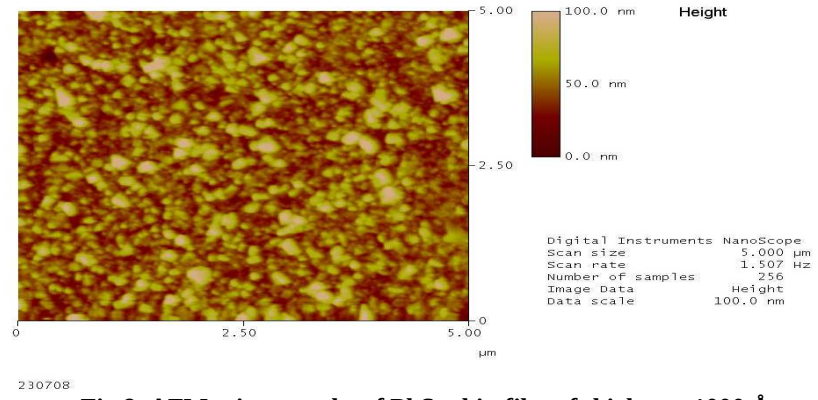

Fig.8. AFM micrographs of PbSe thin film of thickness 1000 Å

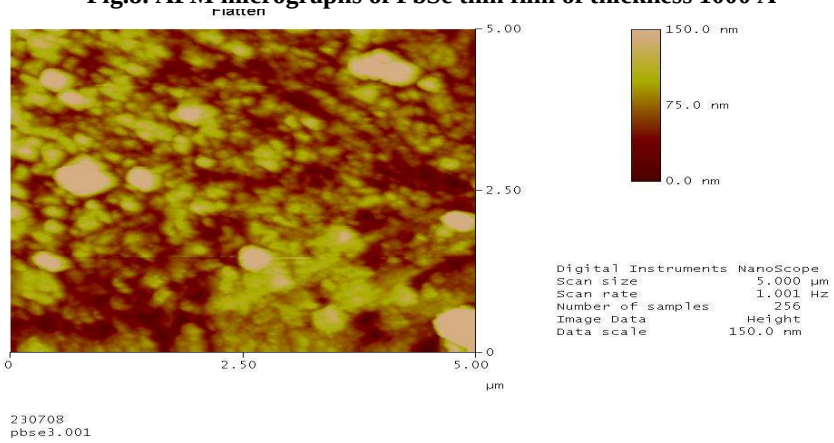

Fig.9. AFM micrographs of PbSe thin film of thickness 2000 Å

Fig. 7, Fig. 8, & Fig. 9, show the two-dimensional view of AFM micrographs of lead selenide thin films having thicknesses of 500 Å, 1000 Å and 2000 Å respectively. The scanning is done over an area of 5µm x 5µm. The micrographs show that the surfaces of the lead selenide thin films consisting of nano scale 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 and roughness of the surface 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

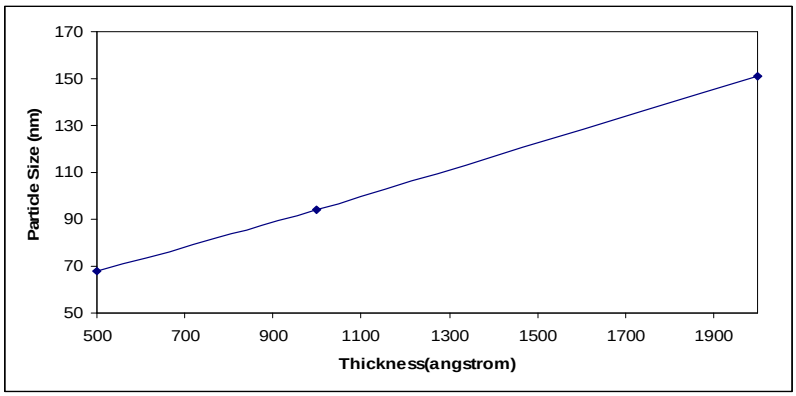

Fig.10. Variation of Particle size PbSe thin films with different thickness

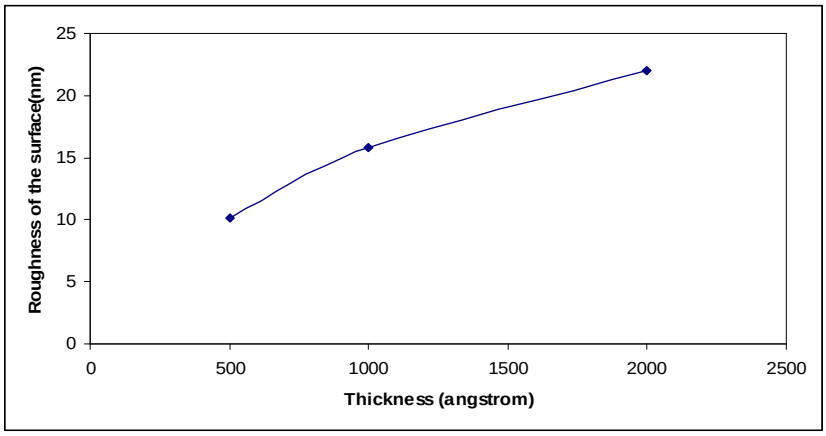

Fig.11. Variation of Roughness of the Surface PbSe thin films with different thickness

Fig.10&11 reveals that particle size and roughness of the surface of the PbSe thin films increases with increase in thickness.

CONCLUSION

The transmittance and absorbance spectra in the range of 2500-5000nm has been taken by using FTIR spectrophotometer. The absorbance spectra show that the material has a high absorbing nature. The observed band gap energy and extinction coefficient has inverse dependence with the film thickness. Absorption coefficient increases as the thickness of the material increases. The surface morphological studies show that the sizes of the particles increase with increase in thickness of the film by means of AFM.

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