Structural and Optical Properties of Lead Selenide Thin Films

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Abstract:

Thin films of Lead Selenide, PbSe, have been prepared at different temperatures by thermal evaporation technique on KCl (100) crystal substrate (prepared by Cleavage method). The structural properties of these films are studied by using X-ray diffraction. It was found that all films have the cubic crystal structure. The lattice constant and grain size were determined. the grain size of these films increased with increasing substrate temperatures. Optical properties also obtained for these films from the spectra of absorbance and transmission of films in the range of(5-15) μm. We have found that there is an effect of Substrate temperatures on the optical band gap of these thin films.

Keywords: structural properties, X-ray diffraction, Lead Selenide, thin films, optical Properties.

المستخلص

حضرت أغشية PbSe بوساطة تقنية التبخير الحراري في الفراغ وترسيبها على قواعد بلوريه من KCl(100) (محضره بطريقة الفلق) عند درجات حرارة قاعدة مختلفة. درست الخواص التركيبيه لهذه الأغشية باستخدام تقنية الأشعه السينيه وقد وجد بان جميع الأغشيه المحضرة تمتلك تركيب بلوري مكعب. تم حساب ثابت الشبيكه والحجم الحبيبي حيث وجد أن حجم الحبيبه يزداد بزيادة درجة حرارة القاعدة .ولدراسة الخواص الضوئية لهذه الأغشية من طيف النفاذية لوحظ تأثير التغير في درجة حرارة القاعدة على فجوة الطاقة للأغشية المحضرة.

1.Introduction

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The study of IV-VI semiconductors such as PbSe has been motivated by using as mid-infrared laser materials [1]. Lead Selenide is very attractive semiconductor material due to its wide verity of applications in photovoltaic absorbers, IR detectors, and photographic [2]. There are several methods for preparing the Selenides such as solid state reaction [3], electrochemical methods [4, 5], microwave assisted preparation [6] and other methods [7,8].

Band gap energies of IV-VI semiconductor which has direct gaps at L point in the Brillion zone are ranging from 0.0 to 0.4 eV. Because the band gaps strongly depend on the temperature, Laser made from these materials exhibit large tuning range [9] making them uniquely suited for high resolution molecular spectroscopy application [10]. PbSe semiconductors are known to be narrow band gap of 0.27 eV at room temperature [11].The effect of the thickness on the structural and optical properties of PbSe thin films prepared on glass substrate was investigated[12].

2.Experimental Method

High purity of Lead Selenide was used for preparing PbSe thin films by thermal evaporation technique. Vacuum evaporator (Varian 3117) was used to prepare PbSe thin films on KCl (100) single crystal substrate at room temperatures, 300°K, 373 and 423°K. The pressure was 10^{-5} torr, the thickness of these films was measured by weight method and approximately found equal to 0.6±0.05 μm. These substrates are prepared by Cleavage method [13]. Temperature controller type CXTA-3000 was used to control the substrate temperature which it was selected at 300, 373, 423 K. Philips (PW1053) X-ray diffractometer was employed for studying the crystal structure of these thin films.

Optical measurements of all thin films samples were carried out using FTIR spectrophotometer type 8900S shimaDZu with the wave number in the range 500-4000 cm^{-1} at room temperature(i.e., wave length 2.5-20 μm).

3. Results and discussion

3.1. X-ray diffraction measurements

X-ray diffraction (XRD) patterns of PbSe thin films which evaporated on KCl(100) substrate at different temperatures, T_s , were shown in Fig.1. XRD analysis showed that the films have highly oriented crystallites with the classical cubic structure with a preferential orientation along the (200) direction which it is agree with the data of Table 1. The degree of preferred orientation increased with increasing the substrate temperature.

Table1: ASTM card No.06-0354 for PbSe powder.

2θ	Intensity	hkl
29.140	100	200
41.683	70	220
49.325	18	311
51.657	20	222
60.414	14	400
66.493	5	331

The inter-planer spacing d_{hkl} was calculated for all planes using the Bragg's law [14]:

$$2d_{hkl} \, Sin\theta_{hkl} = n\lambda , \qquad (1)$$

Where λ, d_{hkl} and θ_{hkl} are wavelength, planner distance of the preferred peak of PbSe and Bragg's angle respectively. hkl and n are order and miller indices.

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From the values of d_{hkl} of each plane, the lattice parameter a of PbSe thin films are calculated from the equation for cubic crystals which is given by:

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

and the grain size D is also can calculated from Debye Scherer's formula [15]:

$$D = \frac{0.9\lambda}{B\cos\theta} \qquad (3)$$

where B is the full- width at half-maximum (FWHM) of the peaks.

Table 2 the shows grain size of PbSe thin films which evaporated on KCl(100) at different substrate temperatures 300, 373 and 423 K. it is clearly see from this table that the effect of the substrate temperature on the grain size. The values of this parameter are increase with increasing in the temperature of substrate, this due to the substrate temperature cause to decrease the density of nucleation centers. Under these circumstances, a smaller numbers of centers start to grow resulting in large grains [16]. The value of lattice constant is found to be equal to 6.132 Å and it was approximately equal to that value of the powder source 6.124 Å. This small difference is due to different substrate temperatures T_s.

Table 2: Grain size of PbSe thin films prepared on KCl(100) substrate.

T(K)	D(Å)
300	205.8
373	235.8
423	275.1

3.2. Optical properties

In Fig.2, we have plotted optical transmission spectrum as a function of wave length for PbSe thin films at three different substrate temperatures, 300, 373, and 423 K. we observe that the effect of substrate temperature on transmittance. The values of the transmittance decrease with increasing in the substrate temperature. By analyzing the optical transmission spectrum, the absorbance coefficient α with photon energy hυ are obtained. Fig. 3 shows the variation of α with hυ at different substrate temperatures. To obtain the values of energy gap of these films, we applied the following relation [16]:

$$\alpha=k(h\upsilon-E_g)^{1/2}/h\upsilon \,, \qquad (4)$$

where k is constant. In Fig. 4, we have plotted $(\alpha h\upsilon)^2$ versus $(h\upsilon)$. The intercept of the extrapolated straight linear portion with energy axis yield the direct band gap value.

In Table 3, Shows the results of the energy gap with different temperatures for PbSe thin films. The effect of substrate temperature is clearly alter on the value of the energy gap. As the substrate temperature increases the value of the energy gap increase. The reason of this behavior is result from the appearance of sublevels. Our results of the energy gap at temperature 300 and 373 K are in a good agreement with the results obtained with other measurements [17].

Table 3: Energy band gap E_g of PbSe thin films prepared on KCl(100) substrate at three different substrate temperatures.

T(K)	E_g (eV)
300	0.265,0.27[17]
373	0.295,0.31[17]
423	0.31

4. Conclusions:

The substrate temperature has an effect on structural and optical properties of PbSe thin films. There is a smaller effect and a clear effect of the substrate

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temperature on the lattice constant and grain size, respectively. The lattice constant found approximately close to that value of the powder source and the grain size increases with increase in the substrate temperature and all films have cubic crystalline structure. In general, the transmittance has similar behavior with variation of substrate temperature. Energy gap of PbSe increases with increase in the substrate temperature.

References

[1] Sachar H. K, Chao I. P. J. Mc Cann and Fang X. M., J.Appl. Phys. ,vol.85, No 10, 15th May(1999).
[2] Mulik R. N , Rotti C. B, Move B. M. , Sutrave D. S. , Shahane G. S., K. M. C. Radkar , Deshmukh L. P., and Hankare R. R., Indian J.Appl.phys.34,903(1996).
[3] Coustal R. , J.Chem. Phys. 38, 277(1958).
[4] Xu D. S, Shi X. S., Guo G. L., Gui L., and Tan Y. Q.. J.Phys. Chem.B104, 5061(2000).
[5] Zhu J.,Koltypin Y., and Gedanken A. , Chem.Mater.12, 73(2000).
[6] Zhu J.,Palchik O., Chen S. , and Gedanken A.,J.Phys.Chem.B104,7344(2000).
[7] Metcalf H. C., Williams J. E., and Caskta J. F., Modern Chemistry; Holt, Reinhart,Winston, Now Yourk, p.54(1998).
[8] Zaho W., Zhu J., and Chen H., Cryst J.. Growth 252, 587(2003).
[9] Walpole J. N., Calawa A. R.,Harman T. C., and Groves. S. H., Appl.Phys .Lett. 28, 552(1976).
[10] Eng R. S., Butler J. F., and Linden K. J, Opt.Eng.19, 945 (1980).
[11] Gautier C., Breton G, and Averous M., J. Electrochem. Soc.145,512(1998)
[12] Prabahar S., Suyanarayanan N., Rajaselcar K., and Srilcanth S ."Lead Seleni films from vacuum Evaporation method - structural and optical chalcogenide Letters, Vol.6,No. S, 203-211(2009).
[13] Ali M. M., M.Sc. Thesis, Basrah University, Basrah, Iraq, (2005).
[14] Kittel C.. "Introduction to Solid State Physics", 6th Edition, 29(1986).
[15] Cullity B. D.. "Elements of X-ray diffraction", 3rd printing, (1967).
[16] Ashour A., Turk . J. Phys. 27,551(2003).
[17] Saloniem H.,"Electrodepositing of PbS, PbSe and PbTe Thin Films". Vtt Publication, Espoo (2000) p.423.

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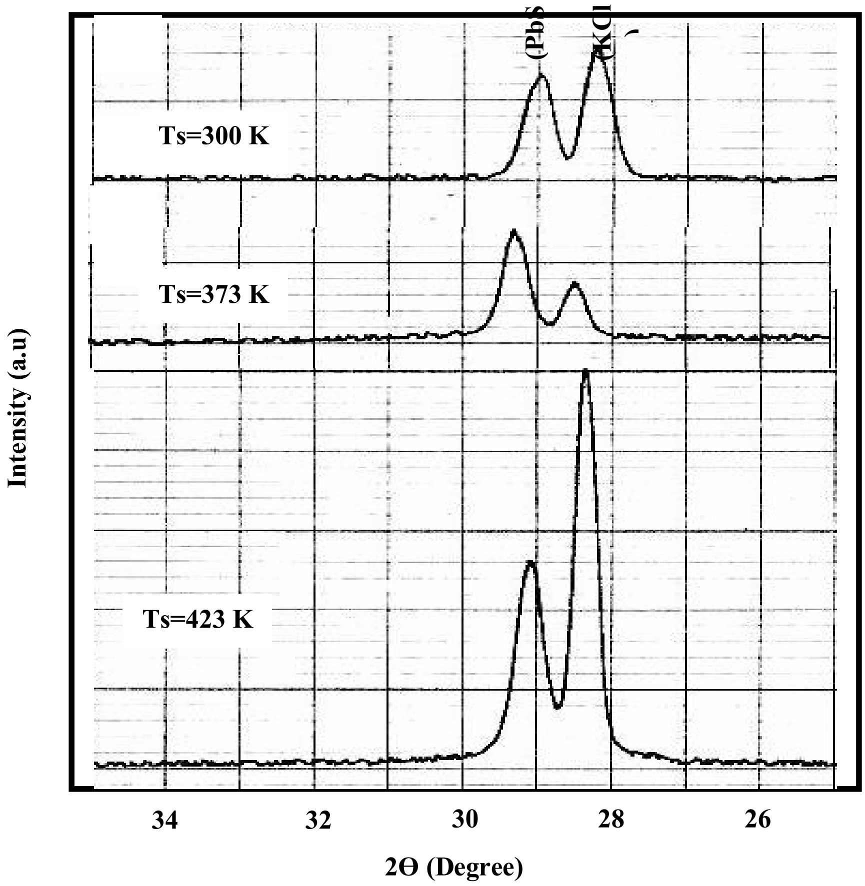

Figure 1:X-ray diffraction of PbSe thin films evaporated on KCl substrate at different temperatures (T_s).

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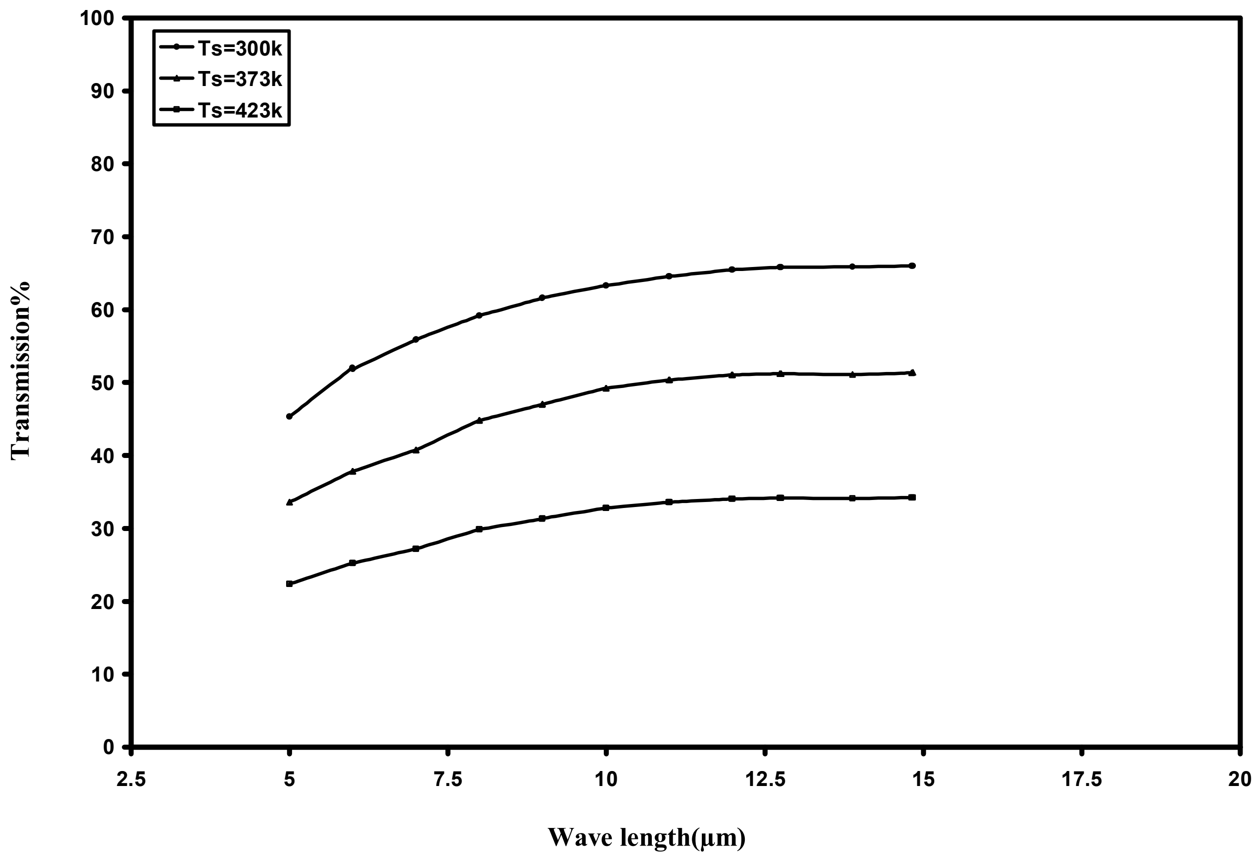

Figure 2: Transmission spectra for prepared PbSe thin films at different substrate temperatures (T_S).

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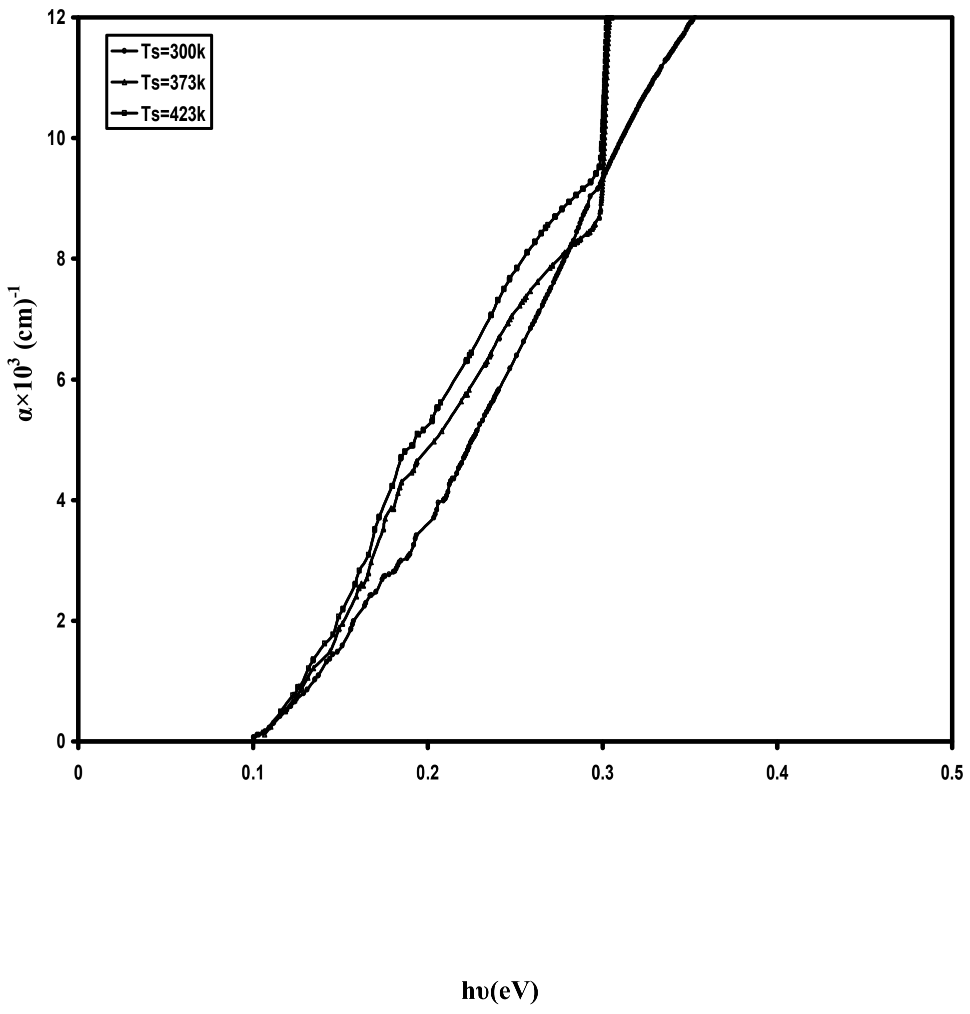

Figure 3: Variation of absorption coefficient(α) with photon energy (hυ) for PbSe thin films evaporated on KCl(100)at different substrate temperatures.

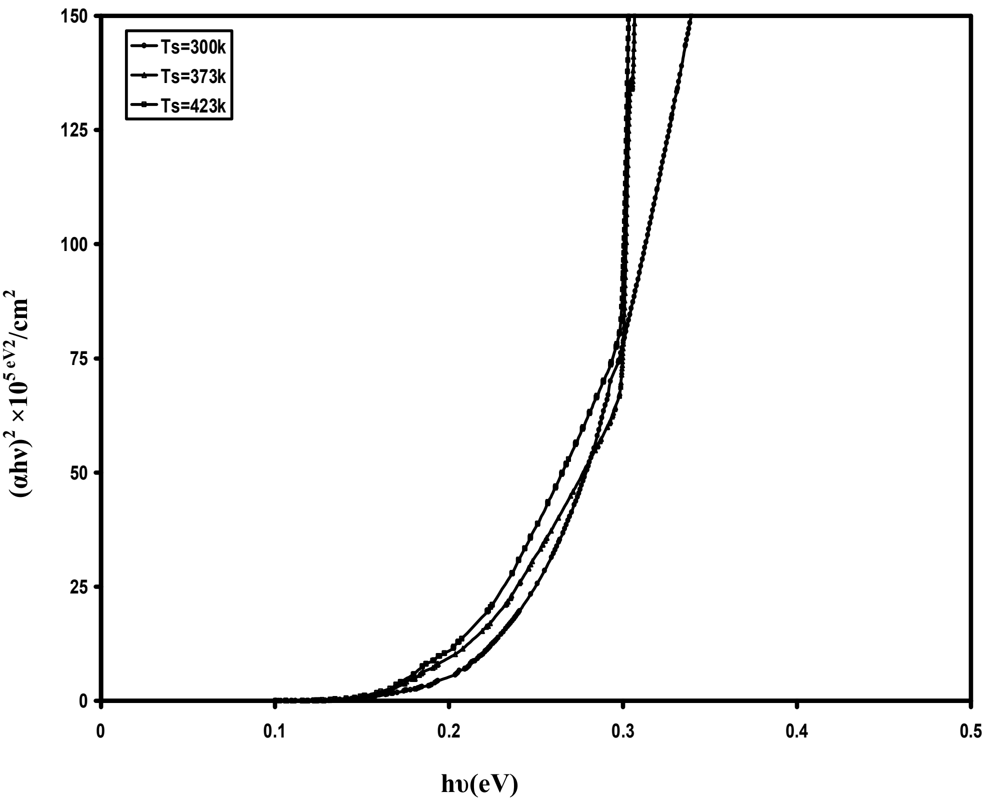

Figure 4: Variation of $(\alpha h\upsilon)^2$ with photon energy($h\upsilon$) for PbSe thin films evaporated on

KCl(100) at different substrate temperatures.