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Structure and optical properties of pbI_2 thin film by thermal evaporation technique

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ABSTRACT

In this search structural, optical and electrical properties were studied by preparing a sample of lead iodide applied to glass bases by thermal evaporation process. The film showed a hexagonal crystalline shape. The value of the energy gap for a sample of 200 nm thickness is 2.9051 eV the intensity is at the plane (003) it's equal 12.5 nm in this research the value of the energy gap was (2.15eV-2.33) eV and the electrical properties were studied for a sample of. The measurements were made for the electrical conductivity, mobility, carrier's concentration and finally the Hall coefficient. The results are ($1.038*10^{-5,}$ $0.6727*10^{+2,}$ $1.009*10^{12}$ and $2.631*10^{6}$) respectively.

1. INTRODUCTION

Many of the researchers worked on choose most important sedimentation methods used for deposition of thin films within a short period of time. Their interest was focused on semiconductors in particular, such as x-ray detectors. [1] Their choice was to use lead iodide to make detectors at room temperature of many specifications, the most important:

Lead iodide is a semi-conductive type P with a high energy gap of 2.3 and a high atomic number with iodine having atomic number = 82 and lead atomic number = 52 so it is used as ionizing radiation detector such as Y ray, X-ray [1, 2, 3] and mass absorption factor (7 µm enough to absorb 90% of the 6-KeV radiation and 1560 µm for 120 Kev) radiation. Lead iodide is very effective at room temperature, [4, 5].

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Lead iodide is an important and promising semiconductor and crystallizes in a hexagonal structure and can be grown from solution, vapor and gels. [6]. Lead iodide is is structural to CdI2 and 20 polytopes have been reported. The poly types of PbI2 are 2H ,4H, 6H, 8H, 12H, 12R, 14H, 18H, 18R, 20H, 20R, 36H ,42R, 48R. The most common type is 2H, which represents 95% polytopes described for PbI2 structure [7]. Recently many research was published on the development of the method of prepared thin films of PbI2 from solutions, vapor, melts and gels. Equally to the recently published results reporting on the influence of rare earth (RE) elements on the quality of materials for radiation detectors [8].

The aim of this work is to prepare a thin polycrystalline lead iodide films by vacuum evaporation method, and studying the optical and structural properties of this material to present preliminary results which in this approach could be a way to develop PbI2 nuclear imaging devices beside the electrical properties. Film thickness was measured after evaporation by optical interferometer method, using He-Ne Laser λ =0.632 μm and the thickness were determined using the formula

Where: d is the thickness of sample, x is fringe width, Δx is the distance between two fringes and λ is the wavelength of He-Ne laser light

2. EXPERIMENTAL WORK

Thin films of PbI_2 have been deposited using resistor heating thermal evaporation system. The system was under vacuum about regularly 2 * 10^{-5} mbar by rotary and diffusion pumps that is monitored by Penning gauge and Pirani gauge.

The figure (1) is shown simple diagram of thermal evaporation deposition system.

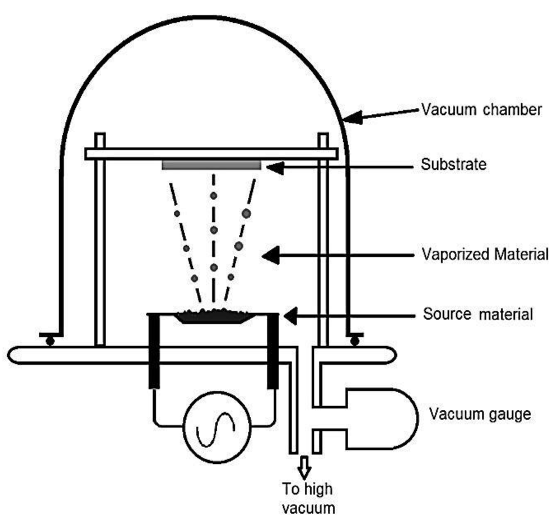

Figure (1): show diagram of thermal evaporation deposition.

The both glass and silicon slides were used as substrate of PbI_2 thin films. All substrates were cleaned by deionized water and ethanol before deposition. After that, they were dried for about 10 minutes. The PbI_2 powder with the purity approximately 99.999% was as source material. This powder was placed on tungsten boat away from substrates was 18 cm. At the required vacuum, the tungsten boat was heating by evaporation current applied on both its ends which was heated to reach temperature greater than the melting point of PbI_2 powder.

The electric properties were measured by electrometer c.Cathlly 65178 the optical properties such as transmission, absorption and optical energy band gap of the PbI_2 thin films were measured by Metertech Inc. SP-8001 UV-VIS Spectrophotometer in UV–VIS wavelengths ranged from 300 to 1100 nm. It was used by X-ray diffraction (XRD) technique (Shimadzu XRD-6000 system with the radiation source of Cu, NF type) to study crystal structure of the thin films. The morphology and roughness of the surface film was analyzed by atomic force microscope (AFM) using Angstrom AA3000.

3. RESULTS AND DISCUSSION

3.1 X-Ray Diffraction and Crystal structure

The structural properties of the deposited thin films were measured by X-ray diffraction analysis using Shimadzu diffract meter (XRD-6000). The crystallite size and micro stress of PbI_2 thin film has been calculated. The Fig. 2 shows the XRD pattern of PbI_2 thin film that was deposited on amorphous silicon, a-Si substrate. In this figure, the hump in the pattern of a-Si is evidence that the substrate used in deposition is amorphous silicon. From XRD pattern of the PbI_2 film, the main diffraction peaks are positions at the planes 003, 004, 006, 009, and 0012, which are located at the diffraction angles 12.73°, 16.98°, 25.58°, 38.65° and 56.13°, respectively.

The crystallite size (D) of the grains and micro strain (ε) were evaluated using Scherer's equation, and the obtained average values are approximately 12.5 nm and 0.003 pa for PbI_2 thin films respectively. The reason the variation of the grain size may be related to the fact that temperature of vaporization of the gradual rise of the boat temperature.

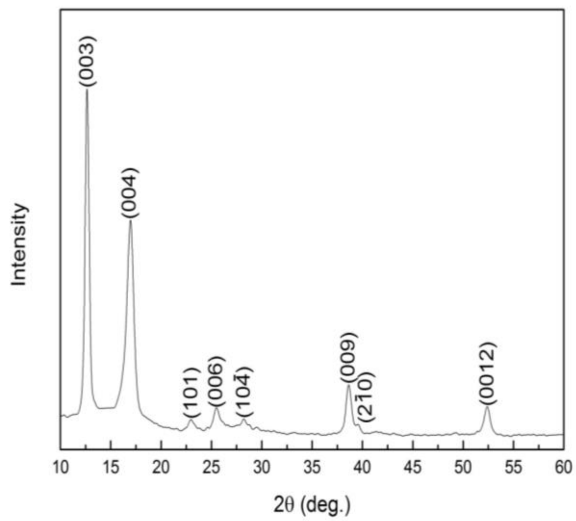

FIGURE 2. XRD patterns of a-Si substrate, PbI_2/a-Si thin film

TABLE 1 the crystallite size and dislocation density with PbI_2 thin film

2θ (deg.)	hkl	Crystallite Size D (nm)	Micro strain ε	SSA (m2/g)was
12.731	(003)	15.13254	0.00239	64.36631
16.9869	(004)	9.72431	0.00372	100.16406
23.0616	(101)	11.20114	0.00323	86.95777
25.5803	(006)	10.34062	0.0035	94.19412
28.2707	(10-4)	9.00655	0.00402	108.1464
38.6569	(009)	13.12545	0.00276	74.20894
39.6341	(2-10)	18.04305	0.00201	53.98345
52.3575	(0012)	12.98714	0.00279	74.99929

3.2 Morphology of Surface Thin Film

"Figure 3" Shows the Atomic Force Microscopy of the PbI_2 thin film, the surface morphology of PbI_2 thin film that is noticed the homogeneous surface; also, there are no cracks and voids on the surface film. Furthermore, it has a surface roughness average of about 5.36 nm and average grain size of the thin film is 33.47 nm. This result means the deposited is extreme smooth and it is less than result in [9]. SSA was calculated by pdf library for XRD device.

Specific surface area (SSA) is a property of solids defined as the total surface area of a material per unit of mass, (with units of m²/kg or m²/g) or solid or bulk volume (units of m²/m³ or m−1). It is a derived scientific value that can be used to determine the type and properties of a material (e.g. soil or snow). It has a particular importance for adsorption, heterogeneous catalysis, and reactions on surfaces.

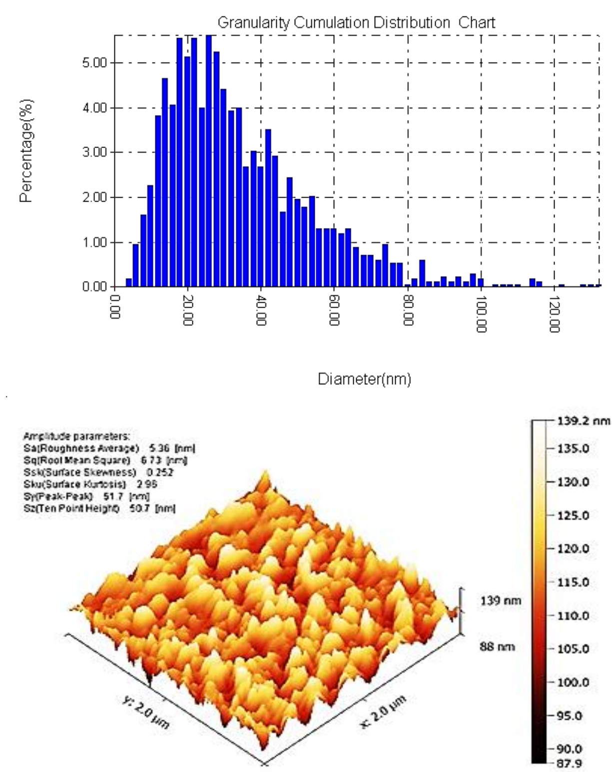

FIGURE 3. Three dimensional AFM topography and grain size distribution of PbI_2 thin film.

3.3. Optical properties

Figure 4 shows the spectral transmittance as a function of wavelength for PbI2 thin films deposited on glass substrate by vacuum thermal evaporation technique. It can be seen that transmittance increases with the wavelength reaching a high transmittance > 80% in the range of wavelength between (575-1100) nm.

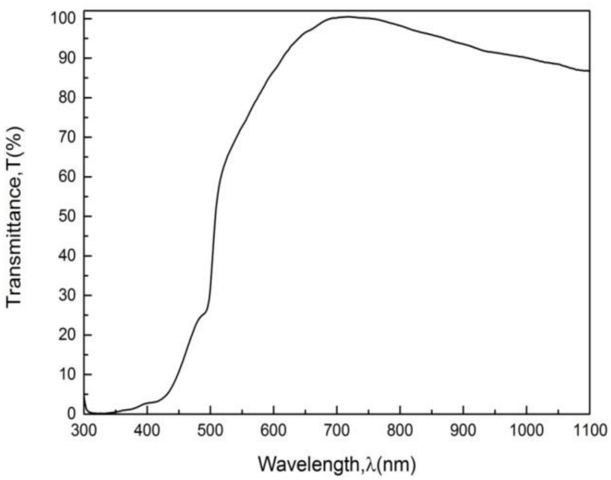

FIGURE 4. Transmittance spectra of PbI2 thin films.

The optical band gap of PbI_2 thin film was evaluated using equation (1) [10]

$$(\alpha hv) = A(hv - Eg)^m \qquad (1)$$

Where *m* equal to ½ and 2 for direct and indirect transitions respectively, A is proportionality constant, Eg is optical energy band gap and (α) is the absorption coefficient. The absorption coefficient was calculated using the following equation [10]:

$$\alpha = \frac{1}{d} ln(T) \qquad (2)$$

Where (d) is the thickness of the film and (T) is the transmittance.

It can be seen from Figure 5, the estimated optical band gap of PbI_2 thin film was found to be 2.9015 eV, and this value is in a good agreement with the work reported by M. Shkir et al [11]**.**

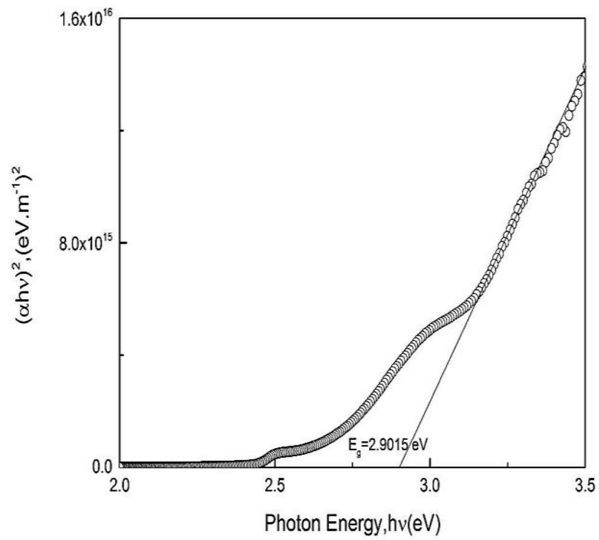

FIGURE 5*:* Optical band gap of PbI_2 thin films

3.4 .Electrical properties

Electrical properties have a crucial role in many applications; this often invites us to study the electrical conductivity to clarify electrical properties. Since the electrical conductivity is a function of the product of the mobility by concentration of charge carriers, and conductivity because both the mobility and concentration of charge carriers rely heavily on compositional properties, therefore, we have tried to link the change in electrical conductivity characteristics with crystalline.

Therefore, in this research, electrical properties were studied for a sample of 200 nm thickness lead iodide which was prepared by thermal evaporation method. The measurements were made for the electrical conductivity, mobility, carrier's concentration and finally the Hull coefficient. The results are shown in the table below.

TABLE 2 the electrical parameters with PbI_2 thin film

Thickness	**200 nm**
Mobility (cm^2/v_s)	**$0.6727*10^{+2}$**
Conductivity (1/Ω cm)	**$1.038*10^{-5}$**
Bulk carrier concentration ($1/cm^2$)	**$1.009*10^{12}$**
Resistivity ($\Omega.cm^2$)	**$1.840*10^4$**
Average hall effect (m^2/c)	**$2.631*10^6$**

4. CONCLUSIONS

In this research, thermally evaporation method was used to deposing Lead Iodide thin films (PbI_2) on glass substrates. A study effects optical and electrical properties of the films was done. X-ray patterns acquired proved the proper phase structure of the PbI_2 films according to ASTM. The better orientation value of (003) plane has the highest value measure among other planes. thickness film is 200 nm, the" grain size" of the PbI_2 films, and the "crystallite size" in the range 15.13254- 12.98714 nm. The" root mean square "roughness of film surface in the film 5.36 nm. About the electrical properties, the PbI_2 films with dfferent thickness always show p-type conductivity

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الخصائص التركيبية والبصرية والكهربائية لأغشية يوديد الرصاص المحضرة بتقنية التبخير الحراري

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الخلاصة:

في هذا البحث تم دراسة الخصائص التركيبية والبصرية وقد تم استخدام جهاز (electrometer c.Cathll 65178) لأجراء الفحوصات الكهربائية لعينة من يوديد الرصاص المرسب على قاعدة من الزجاج بواسطة عملية التبخير الحراري وقد اظهرت الاغشية الشكل البلوري السداسي للعينة وبلغت قيمة فجوة الطاقة لعينة من يوديد الرصاص ذات سمك 200 nm هي (2.9051eV) , وان الحجم الحبيبي عند المستوي (003) لبوديد الرصاص هو 12.5 nm .وقد تم فحص كل من التوصيلية والتحركية بالإضافة الى تركيز حاملات الشحن ومعامل هول وكانت النتائج كالاتي على التوالي ($1.038*10^{-5}$, $0.6727*10^{+2}$, $1.009*10^{12}$, $2.631*10^{6}$) .