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# Structural and Optical Properties of $PbI_2$ Thin Films to Fabricate Perovskite Solar Cells

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**Abstract.** Recently, lead iodide is the most materials employment in the perovskite solar cell application. This paper has studied the character of preparation, structural and optical properties of $pbI_2$ materials. Structural properties are included investigation of the measurements X-Ray Diffraction (XRD), Scan Electron Microscopy (SEM), Fourier Transform InfraRed spectroscopy (FTIR) and Atomic Force Microscopy (AFM) tests to the $PbI_2$ thin films samples. Optical properties are included the investigation UV-Vis test of the thin film samples deposited on glass substrates and investigated the Absorption, Transmittance and evaluated energy gap ($E_g$ = 2.3 eV).

## Introduction

At last decade, Lead Iodide (PbI2 ) is to be a very promising material with large technological applicability as Perovskite photovoltaic solar cells, an addition, X-Ray and γ–ray detectors at room temperature [1] [2] [3] [4] [5] [6]. Lead-iodide is an important material in the preparation of solar perovskite cells that have been widely studied by many researchers around the world, and the Power Conversion Efficiency (PCE) reaches more than 20%, and recently [4], $PbI_2$ is a wide optical bandgap energy (2.3–2.6 eV) semiconductor materials with elements of high atomic number, density of 6.2 g/cm and high resistivity ($10^{13}$ Ωcm) [7]. The wide bandgap makes possible for low noise influence of the $PbI_2$ detectors at temperature 30 ºC or above [7]. One of the apparent disadvantages of PbI is the low mobility of its charge carriers, 8 cm /Vs for electrons and 2 cm /Vs for holes, Therefore, in order to advance the electrical properties, the trapping operation (characteristics and the mobilities) should be improved [7]. The procedure method of preparation $PbI_2$ powder or thin films samples and characteristics of structural and optical properties were described in the present work.

## Experimental

In the research, the Lead Ioded ($PbI_2$) was prepared in the laboratory according to the[8] and the following reaction of equation 1:

$$Pb(NO_3)_2 + 2KI \rightarrow PbI_2 + 2K^+ + 2NO_3^- \quad (1)$$

The $Pb(NO_3)_2$ interacted with potassium iodide (KI) at a ratio of 1:2 in water at 70 ºC. Sample A, 10g of the $Pb(NO_3)_2$ were dissolved in 25ml of deionized water at temperature 50 ºC. SampleB, 10g of the Potassium Iodide (KI) were dissolved in 25ml of deionized water at temperature 50 ºC. Mix sample A on sample B at 70ºC on the hot stirrer, then we obtained yellow precipitator indicated to Lead Ioded, $PbI_2$, as shown in figure (1). The prepared $PbI_2$ was washed with distilled water 4–5 times. Followed by, drying at 100 °C, a yellow powder is formed, which is placed overnight in a vacuum oven before use. To obtain the $PbI_2$ precursor solution, we dissolved 0.153g of the powder

$PbI_2$ in 10 ml of anhydrous N, N DiMethyl Formamide (DMF) (Sigma Aldrich). Thin films of $PbI_2$ samples were prepared with spin-coated technique at speed 2000 rpm at 20 sec. and annealed on a hot plate at the temperature of 100 ºC.

**Fig. (1)** Is depicted the precipitator $PbI_2$ in deionized water.

**Characterization of the Film:**

The morphology of the film was investigated by an Atomic Force Microscopy (AFM) (AA 3000 Scanning probe microscope, Angstron Advanced Inc.). The transmittance of $PbI_2$ film coated was measured in the wavelength range of (190 - 1200) nm using a (SPECTRO UV/VIS Double Beam (UVD-3500) Labomed, Inc.). A blank sample of the substrate was used as a reference in the measurement of optical transmittance and thickness. Composition and crystal structure studies were investigated by X-ray diffraction (XRD-Shimadzu 6000, Cu-K). The structures of the $PbI_2$ crystals studied by images of Scanning Electron Microscope (SEM) (Bruker Nano GmbH, Germany). The transmittance FTIR of the powder samples is measured in the wavenumber at a range of (0 - 4000) $cm^{-1}$ by using a (SPECTRO FTIR TENSOR 27). A blank sample of the substrate is used as a reference in the measurement of optical transmittance.

**Basic Theory:**

The optical properties of $PbI_2$ thin films were studied. The Absorption coefficient (α), was measured as a function of the energy of the photon incident. Equation (2) is based on the Beer-Lambert law for optical absorption, where $I_o$ is the intensity of the incident light and I is the intensity of the transmitted light of the film with thickness (t), Absorbance (A), and the Absorption coefficient (α) which shown in the following equation[9]:

$$\boldsymbol{\alpha = \frac{1}{t} * ln\left(\frac{I_o}{I}\right) = 2.303 * \frac{A}{t}} \quad (2)$$

We calculated the indirect optical band gap of the thin film $PbI_2$ from the equation (2) [9][1] and [10]:

$$\boldsymbol{h\nu * \alpha = B * \left[h\nu - E_g\right]^2} \quad (3)$$

Where, h is the Planck constant, (α ) is the absorption coefficient, ν is the light frequency, Eg is the optical energy gap and B is empirical constant [10].

**Results and Discussion**

**Structural Properties:**

Figure 2(a) depicts the XRD results for $PbI_2$ coated film on the glass substrate by employment spin coated technique. The investigation compared the XRD pattern of the $PbI_2$ thin film with the JCPDS file. On the basis of the XRD results, it appeared that the $PbI_2$ thin film had a hexagonal

crystalline structure with constant lattice (a=4.67A°, c=7.52 A°) at diffractions (001), (101), (102), (110), and (103) identified of the Ref JCPDS file #07-0235. There is complete agreement between XRD spectra and Ref of JCPDS file for the XRD pattern of PbI2 synthesized powder, indicating that the PbI2 synthesized powder in the lab is the same as the standard Ref of JCPDS file #07-0235, as shown in figure 2(b). Figure (3) is illustrated electrons charges density at resolution 0.5A° in the plane (102) of the hexagonal structure of $PbI_2$ crystalline which are created via Visualization for Electronic and Structural Analysis (VESTA) program. The maximum and minimum values of the charge density of saturation levels at the plane (102) of the scale bar are (8.21 and 7.93)% of the total electron charges density, respectively, as shown in figure (3).

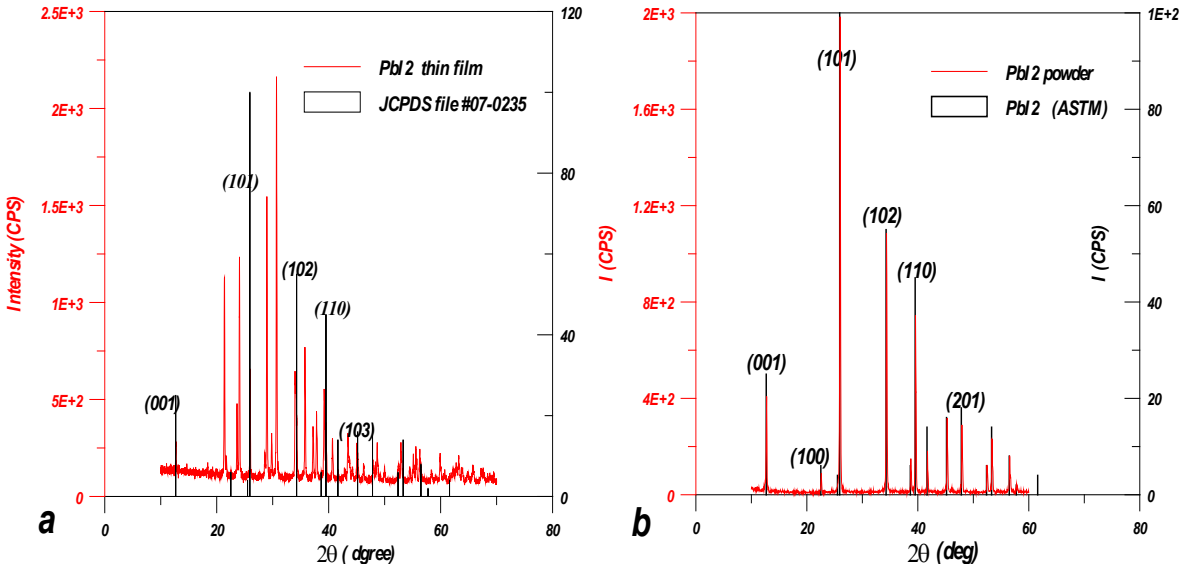


**Fig. (2)** Depicts XRD pattern of (a) the coated $PbI_2$ thin film and (b) the synthesized $PbI_2$ powder, comparative with Ref of JCPDS file #07-0235.

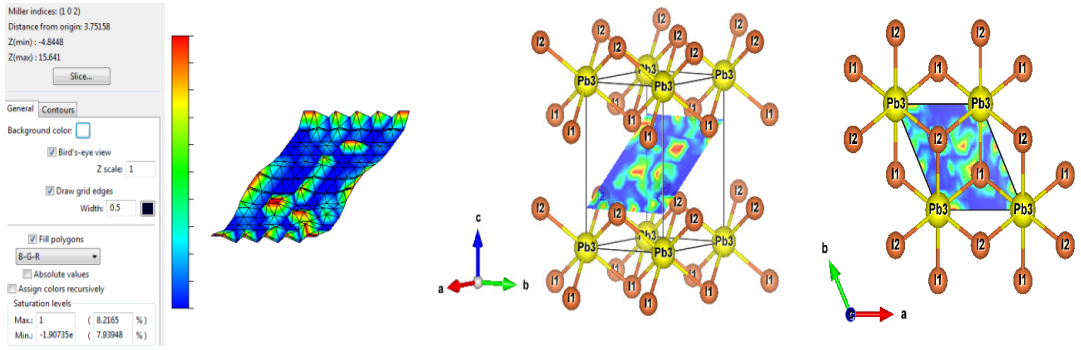


**Fig. (3)** Is illustrated electron charge density in the plane (102) of hexagonal structure of $PbI_2$ crystalline which are created via VESTA program.

Figure (4). is illustrated IR spectra of the powder of the lab preparation $PbI_2$ sample. The peak at frequency 1627 referred to the band Pb-I, as shown in figure (3). Dinghan Shen, et al. are mentioned that ascribed this result to a broad band located at 1627 $cm^{-1}$ introduced by $PbI_2$.[11].

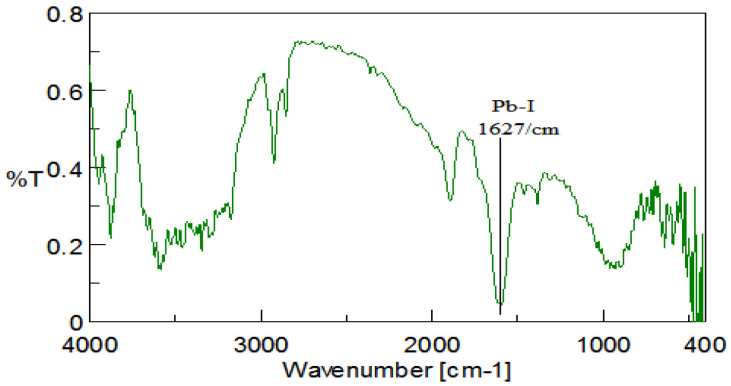


**Fig. (4)** Is depicted IR spectra of the prepared sample powder of the $PbI_2$.

Figure (5). depicts the SEM images of $PbI_2$ thin film sample which is prepared of spin-coated technique with parameters of preparation conditions at speed (2000 rpm), time (15sec) and followed by annealing at a temperature (100°C). The SEM images are measured with parameters of testing conditions at SEM High Voltage (10kV), SEM Magnification, (100,50 and 30)kx and Scale bar, (200,500 and 1000)nm. It may be observed that the SEM images refer to form the rods and sheets configurations. An addition SEM test, the quality of the PbI2 film is further evaluated by Atomic Force Microscopy (AFM), as shown in figure (6). The Lead Iodide (PbI2) film possesses the characteristics of full surface coverage and being pinhole-free on the substrates. In addition, the porous nanostructure presented in the PbI2 film vanished of crystals which form at diameters plates sizes less of 70 nm, as shown in figure 5(b). The Root Mean Square (RMS) roughness of the film is calculated to be (6.47) nm, Roughness Average is (5.5)nm, Peak-Peak is (22.9)nm and Average Diameter is (86.80)nm in the range of (1.465)µm ×(1.48)µm, as shown in figure (6) and table (1), which is better than the previously reported that root mean roughness RMS of the films PbI2 are 19.3 and 17.8 nm, [6]. The smooth surface morphology is an indication of the effective conversion of the porous PbI2 nanostructure into perovskite thin films of the plates or rods as confirming in SEM images in figure (5).

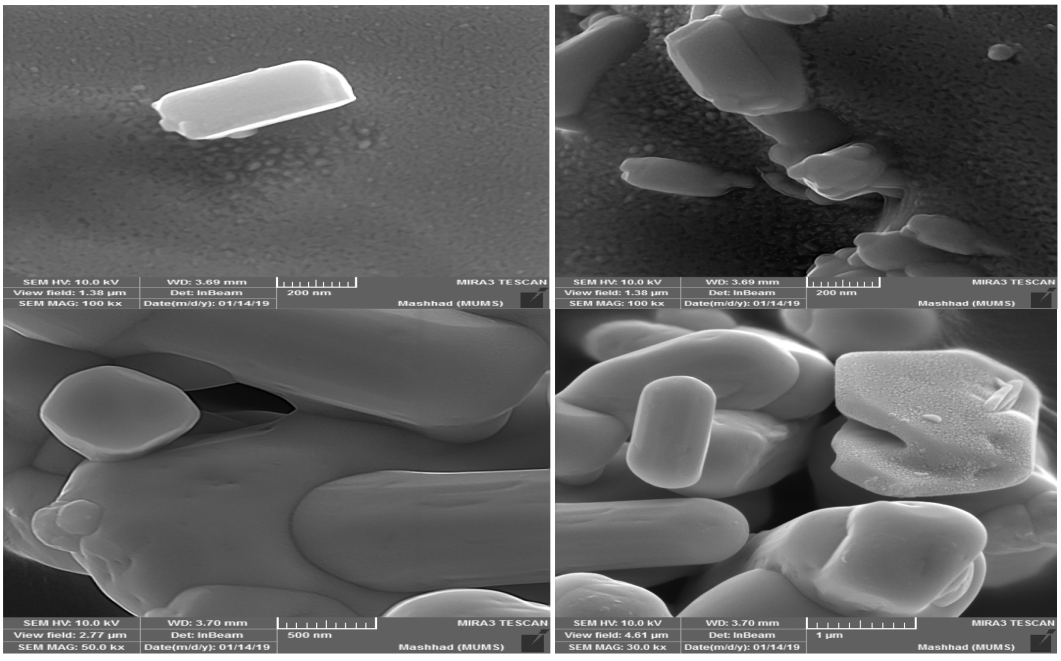


**Fig. (5)** Explains the top view SEM images of $PbI_2$ thin film sample.

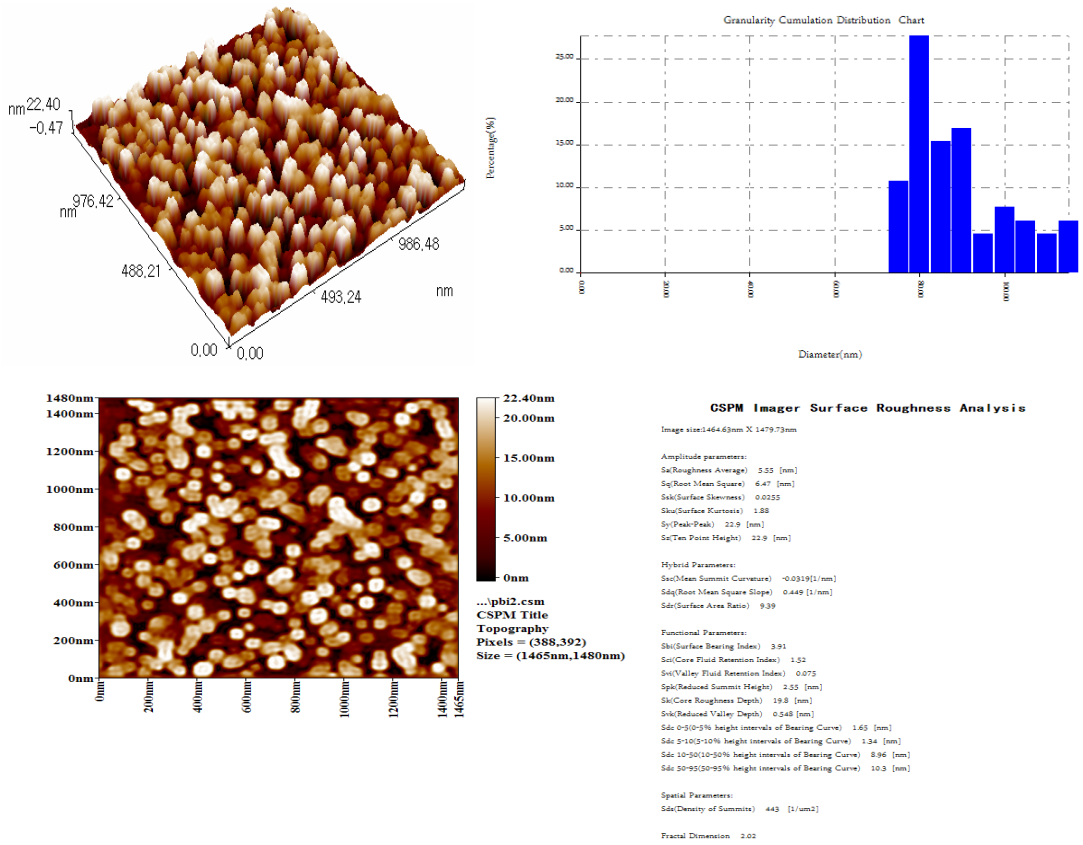


**Fig. (6)** Explains the top view AFM images of $PbI_2$ thin film sample.

## Optical Properties:

Figure 7(a) is explained the absorption of Lead Iodide ($PbI_2$) thin film and the sample is measured in the wavelength range (350-1100) nm using a (SPECTRO UV/VIS Double Beam (UVD-3500) Labomed, Inc.) with a glass substrate as a reference sample. Figure 7(b) is depicted the Plot inset of $(\alpha hv)^{0.5}$ versus photon energy (E) for the coated thin film $PbI_2$ on glass substrates. Indirect optical band gap energy (Eg) for Lead Iodide ($PbI_2$) material is reported by [1]. (Eg) of the sample is determined by fitting the absorption data to the direct transition equation (4). The optical band gap value is obtained by extrapolating the linear part of the curve $(\alpha hv)^{0.5}$ as a function of photon energy, hv, intercept the (hv) axis at $\alpha = 0$. The value estimated of Eg is (2.3 eV), as shown in figure 7(b) and table (1). The sample thickness was confirmed as an important parameter to estimate Eg which was measured ($t = 40$ μm). $PbI_2$ is a wide bandgap energy (2.3–2.6 eV) semiconductor composed of high atomic number elements ( $Z_{Pb} = 82$, $Z_I = 53$), with high resistivity ($10^{13}$ Ωcm) and density of 6.2 g/cm$^3$[12] [7]. The structural properties parameters of XRD studies with AFM test report studies and optical properties studies parameters of $PbI_2$ thin films samples were inserted in the table (1).

**Table (1)** Explains the parameters of the structural and optical properties of $PbI_2$.

| Structural properties | | | | Optical properties | |
|---|---|---|---|---|---|
| Hexagonal Structural | | AFM Test | | | |
| a | 4.69A° | RMS | 6.47nm | Eg | 2.3 eV |
| c | 7.52A° | R.A. | 5.5nm | | |
| VESTA program | | P.P. | 22.9nm | | |
| a | 4.68942 A° | A.D. | 86.8nm | | |
| c | 7.50316 A° | | | | |

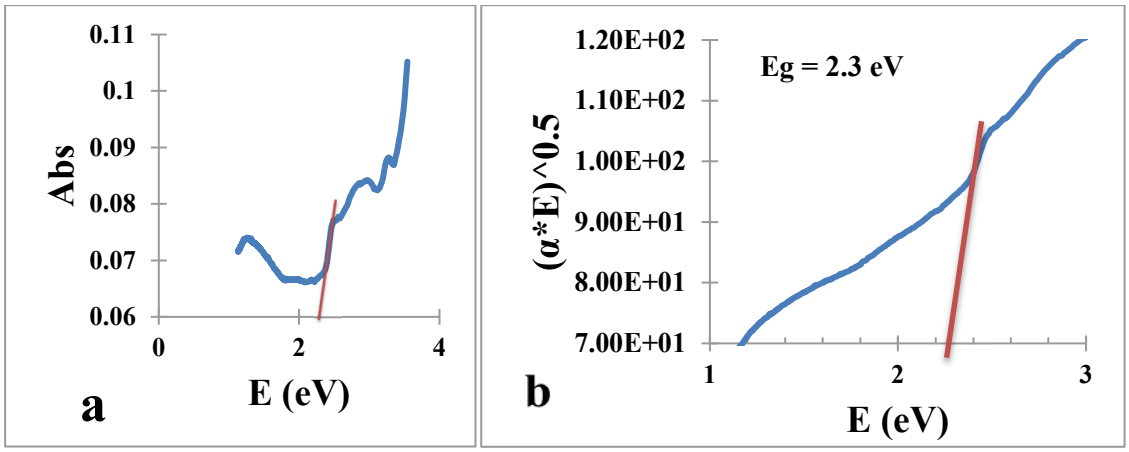


**Fig. 7**(a) Depicts the absorption and (b) energy gap of Lead Iodide ($PbI_2$) thin film.

**Conclusions:**

From the results obtained in this work, the indirect band gap energy for $PbI_2$ was estimated at 2.3 eV. An addition, the expediency agreement between AFM results and SEM results was observed in the structural investigation of the $PbI_2$ thin films samples. Although, it can be observed that un agreement between the XRD patterns of $PbI_2$ powder sample and $PbI_2$ thin film sample. Clearly, new peeks were appeared, probably, due to an effect annealing process. Moreover, the VETA program was enhanced the XRD pattern and lattice parameters estimated of hexagonal structural of XRD studies of $PbI_2$ samples. Consequently, the present work is expounded the simple experimental procedure to prepare $PbI_2$ material which is worth further study and can be applied to fabricating new perovskites as well as other planar substrates of photovoltaic perovskites solar cells.

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