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Study of Some Properties of PbI_2 Deposited on Porous Silicon Using Thermal Evaporation Technique for Many Applications

Suha G. Ali*, Mohammed S. Mohammed, Fatima I. Sultan

Department of Applied Sciences, University of Technology – Iraq

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****Corresponding Author:***
Suha G. Ali
as.18.05@grad.uotechnology.edu.iq

Abstract

The present work is a study of some properties of PbI_2 deposited on porous silicon (n-PSi) by using the thermal evaporation technique. X-ray diffraction, scanning electron microscopy, UV–Vis spectrophotometer, and FTIR analysis were used to characterize the structural, optical, and morphological properties of n-Psi. X-ray diffraction showed that the PbI_2 film has a hexagonal polycrystalline structure, while FE-SEM images showed porous silicone in Photoelectrochemical etching, the pore distribution is irregular and the pore refers to the increased surface area of the silicon. SEM images of pbI_2 film showed that particles were scattered and resembled gravel in size. The estimated optical energy value of thin films of PbI_2 was 2.6 eV. PbI_2 film has lower transmittance values at short wavelengths, but as the wavelength increases, the transmittance values gradually increased. The greatest transmittance value was 0.88. From FTIR analysis, chemical bonds were determined between porous silicon and PbI_2.

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1. Introduction

Lead Iodide (pbI2) has emerged as a promising material with broad technical applications, including Perovskite photovoltaic solar cells, X-ray, and γ–ray detectors at room temperature [1-6]. Lead-iodide is an important ingredient in the fabrication of solar perovskite cells, which have been extensively explored by numerous researchers across the world and have recently achieved a Power Conversion Efficiency (PCE) of more than 20% [4]. Lead iodide is a semi-conductive type P with a high energy gap of 2.3-2.6 eV depending on the deposition process, and a high atomic number with iodine having atomic number = 82 and lead atomic number = 52, making it useful as an ionizing radiation detector [3], it also can be utilized in medical imaging, nuclear detection and photosensitivity semiconductor metal applications [7]. Generally, PbI2 can be crystallized by a hexagonal lattice layered form. Its hexagonal closed-pack (HCP) crystal is made up of covalently bound layers of I–Pb–I that are piled on top of one another by weak van der Waals bonds perpendicular to the crystal c-axis [00l]. The anisotropic features of pbI2 crystals are due to this layered structure, which may lead to the formation of numerous polytypic structural changes. [8]. Porous silicon (PS) has recently been a matter of significant investigation, owing to its photoluminescence features and possible uses in photovoltaic devices, chemical sensors, and biological sensors [9, 10]. The idea of etching silicon surfaces has gained a lot of importance in semiconductors and solar cells since it helps to improve and produce devices that have a wide range of applications. The etching process has progressed to nanotechnology, where the material acquires new properties as it reaches atomic dimensions and is governed by quantum rather than classical rules [11]. Porous silicon (PSi) is made up of a network of silicon wires and voids that are nanoscale in size. It is made in a variety of ways, including photoelectrochemical etching of the surface of crystalline silicon in an aqueous solution of (HF)acid, with carefully controlling the preparation conditions (etching time - slice specifications - acid concentration and current density) to obtain a suitable crystal structure from porous silicon with various layers of porosity [12,13]. This work aims to prepare lead iodide films deposited on porous silicon by a vacuum evaporation method, it also studies some properties of this material to present preliminary results for a variety of applications. In (2018), Rana Kadhim Abid alnabia, Malek A.H. Muhi et al have prepared lead iodide that was applied to glass bases by a thermal evaporation process, they also studied optical and electrical properties. 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 equals 12.5 nm. The electrical properties were studied for the measurements of electrical conductivity, mobility, carrier concentration, and finally the Hall coefficient. The results are (1.038*10- 5, 0.6727*10+2, 1.009*1012 and 2.631*106), respectively [14]. K. I. HASSOON, M. S. MOHAMMED, et al, (2019) prepared porous PbI2 thin films to be investigated. Various thicknesses of lead iodide thin films were prepared by the fast thermal evaporation technique (TET). Scherrer's analysis indicated that grain size extends from about 8 to 18 nm. Scan electron microscopy (SEM) revealed high porosity of pbI2thin films. UV-Vis spectroscopy and diffuse reflectivity were used to calculate the optical band gap. The two methods indicated that the PbI2 prepared by TET has a direct optical band gap (about 2.5 eV) with the Urbach tail width of the order 0.76 eV. [15]. Kawther A. Khalaph et al. (2020), studied the character of preparation, and structural and optical properties of pbI2 materials. Structural properties are included in the investigation of measurements. X-ray Diffraction (XRD) revealed that the pbI2thin film had a hexagonal defect and diffusion crystalline structure with constant lattice (a=4.67A^{o}, c=7.52 A^{o}). Scan Electron Microscopy (SEM) images referred to the formation of rods and sheet configurations. The peak at a frequency of 1627 refers to Fourier Transform Infrared spectroscopy (FTIR), the band Pb-I, and Atomic Force Microscopy (AFM). Lead Iodide (pbI2) film possesses the characteristics of full surface coverage and is pinhole-free on the substrates. UV- Vis tests of thin-film samples deposited on glass substrates were used to examine and evaluate optical parameters such as absorption, transmittance, and the energy gap (Eg = 2.3 eV) [16].

2. Experimental Procedures

2.1. Preparation of Porous Silicon

The substrate was a crystalline wafer of n-type Silicon with a resistivity of (5) Ω.cm, a thickness of 500 m, and an orientation of 100. The substrates were cut with (1.5 x 1.5cm^2) areas. After chemical treatment, 0.1µ m thick Al layers were formed on the backsides of the wafer using an evaporation method. Photoelectrochemical etching was then carried out at room temperature by employing a platinum electrode in a mixture (1:1) of HF (45%) and Ethanol (99.99%). The light source was a Halogen lamp with a light intensity of 20mW/cm^2 to ensure homogeneity of the etch layer, current of 14mA/cm^2 was applied for 8 minutes as shown in Figure 1. The etched area was (0.785 cm^2) as shown in Figure 2.

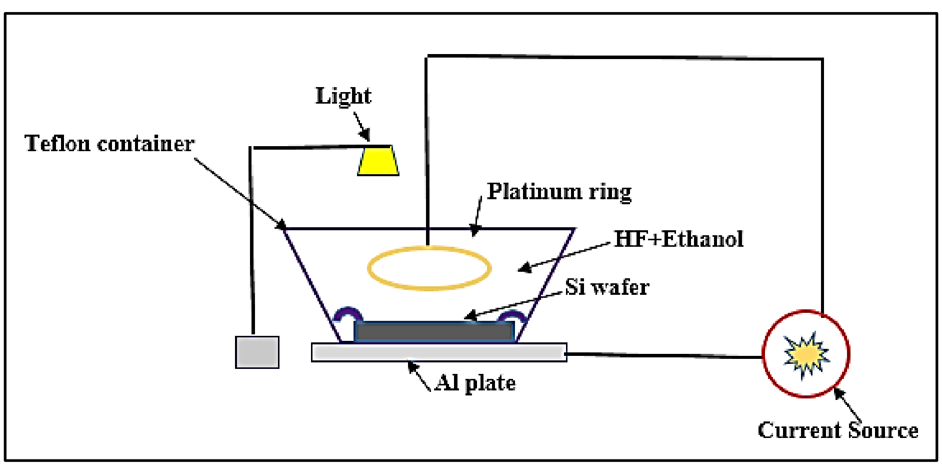


Figure 1: The schematic diagram of the Photoelectrochemical etching method.

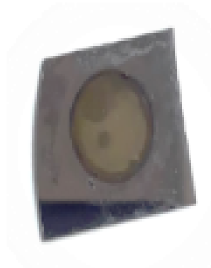


Figure 2: Porous silicon sample.

2.2. Preparation of PbI_2thin Film

PbI2 films of 200 nm thickness were deposited on a cleaned glass and PSi substrate by the thermal evaporation method at a 10-5 Torr vacuum using a high vacuum coating apparatus (Edwards type E306A). The distance between the source and the substrate was roughly 18 cm inside the vacuum chamber, where a molybdenum boat was utilized to transport PbI_2 powder. Figure 3 a & b shows the thermal evaporation procedure and the PbI_2 thin film after it has been deposited on the PSi substrate, while Figure 4 shows the cross-section image of the heterojunction that has been prepared.

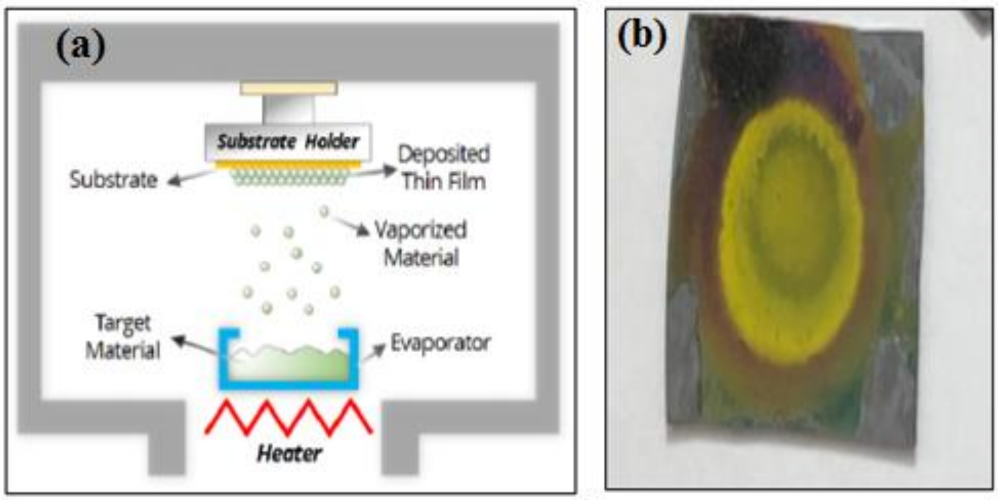


Figure 3: (a): Scheme of thermal evaporation method, and (b): PbI_2 thin film on PSi substrate.

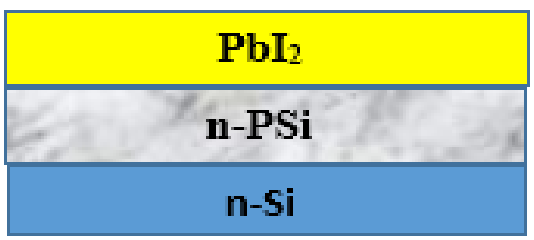


Figure 4: Across-section view of the prepared n-Si/n-PSi/PbI_2 heterojunction.

3. Characterization

PbI2 and PSi film were characterized by utilizing characterization techniques, namely: X-ray diffraction (XRD), Scanning electron microscopy (SEM), UV-Vis, and Fourier transform infrared spectroscopy (FTIR).

4. Results and Discussion

Figure 5 shows X-ray diffraction of crystalline Si and n-PSi materials. Blue plots for n-Si and red drawings for PSi were produced by anodization with a current density of 14 mA/cm^2 and an etching period of 8 minutes. When compared to the peak of n-type porous silicon (n-PSi), the crystalline Si peak has a higher intensity value. Even after the etching procedure, the etched silicon retains its single crystal structure, but due to strain, it slightly moved to a small diffraction angle (2θ 69.428^o and 69.381^o), orientated exclusively along the 400 direction, resulting in a modest expansion in the lattice parameter [17, 18].

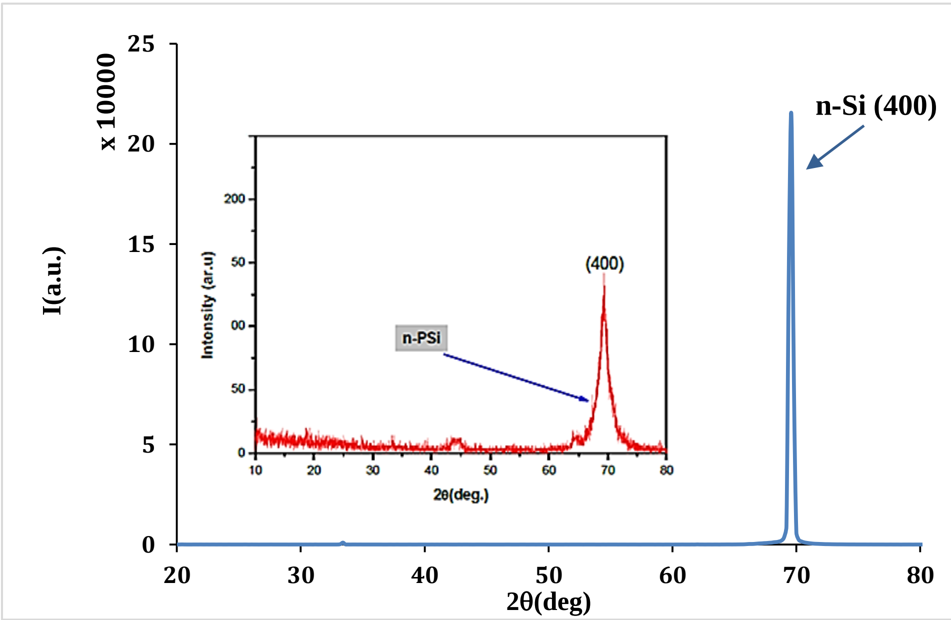


Fig.5. XRD spectra of n-type Silicon (n-Si) and porous silicon (n-PSi) (prepared with14 mA/cm^2 etching current density at etching times 8 min).

The Cu-K target with wavelength 1.54060°A was used to achieve X-ray diffraction of PbI_2 film that was produced on PSi substrate (using XRD Analysis XRD- 6000). Figure 6 reveals the principle diffraction peaks at corresponding planes 001, 101, 002, 202, 003, 210, and 004 at the diffraction angles 12.73°, 23.98°, 25.58°, 28, 38.65°, 39.7, and 52.13°, respectively.

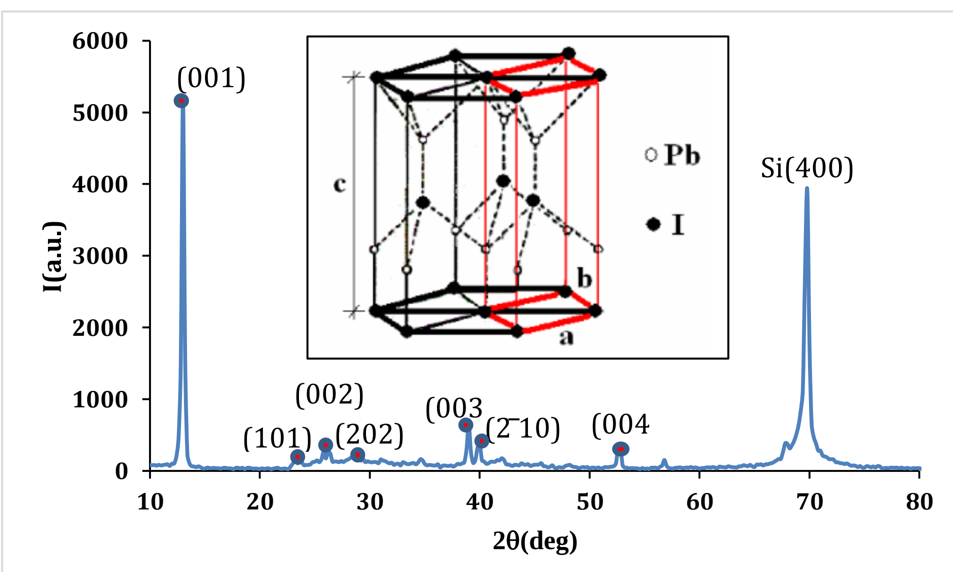


Figure 6: XRD pattern for PbI_2 thin film prepared by vacuum thermal evaporation method.

Similarly, the figure reveals the sharp and narrow peak at the angle of 69.8^{o} for the porous silicon layer with orientation (004). PbI_2 thin film is polycrystalline and has a hexagonal structure, it was indicated in the JCDPS card about [14]. Scherer's Formula (Eq.1) was then used to calculate the average crystalline size that was around (18.28) nm [14-20] when θ, and β in radian angle, and k is a shape factor that equals 0.9.

$$\boldsymbol{D = \frac{k\,\lambda}{\beta\, cos\theta}} \tag{1}$$

D: crystalline size, (λ): wavelength for x-ray (1.5406$\dot{A}$),β: is the full Width at half maximum, and θ: is a degree of diffraction [21]. Figure 7a shows the SEM image of the PSi surface prepared at a current density of 14 mA/cm^2 for an 8-minute etching duration. The bright parts in both photos indicate Si structures, while the dark regions represent pores. The sponge-like structure of the porous silicon layer is readily visible in the images. Pores of varying sizes and spherical forms exist in the prepared layer. Pore diameter ranges from 100 to 200 nanometers. Figure7b shows the SEM images of PbI_2 film on porous silicon deposited by thermal evaporation, where it was observed that the particles scattered on the surface in a heterogeneous manner, mimicking gravel forms, resembling gravel shapes, and their different sizes do not exceed 100 nanometers.

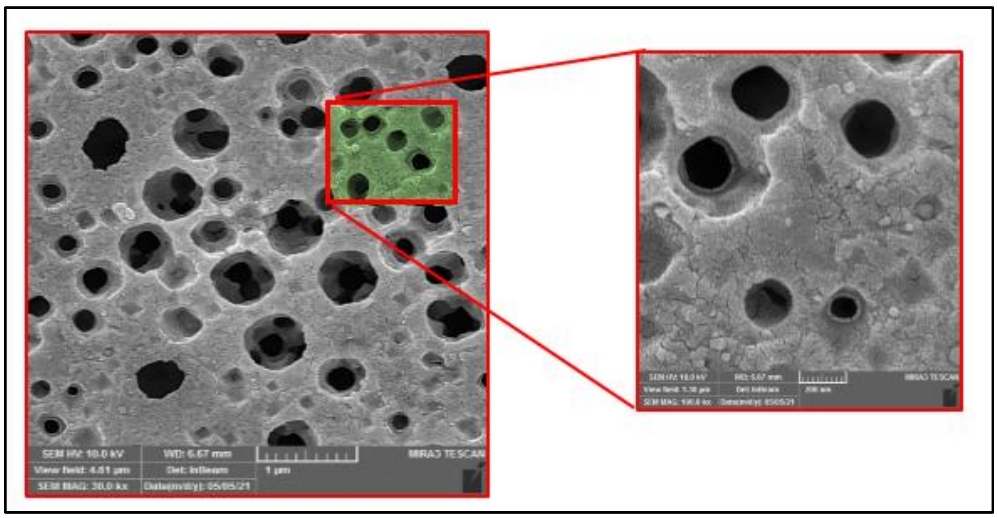


Fig.7a. SEM images of porous silicon samples were prepared with an etching time of (8mins.) at a current density of 14 mA/cm^2.

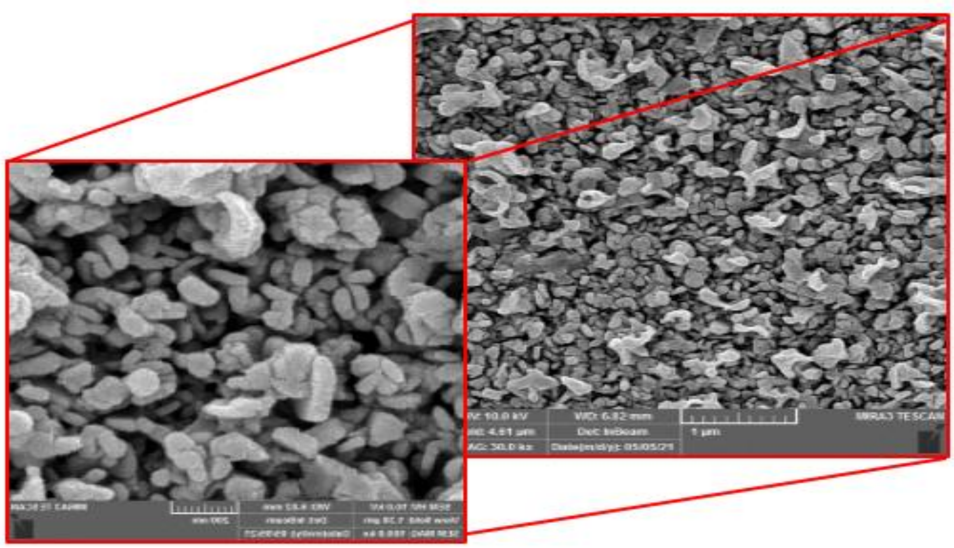


Figure7b.SEM images for PbI2 thin film surfaces on porous silicon.

The optical properties were recorded by using a UV-Vis spectrophotometer (Metertech SP8001). Figure 8 shows the transmission spectra of PbI2 films deposited on a glass substrate using thermal evaporation as a function of wavelength (200-1000) nm. The film's structure, preparation, film thickness, and deposition circumstances all have a significant impact on transmission. PbI_2 film has lower transmittance values at shorter wavelengths, but as the wavelength increases, the transmittance values gradually increase. The greatest transmittance value was 0.88, which is ideal for optoelectronic devices, particularly solar cell window layers. Furthermore, a dramatic drop at the band's edge refers to PbI2 film crystallinity, which is consistent with XRD data.

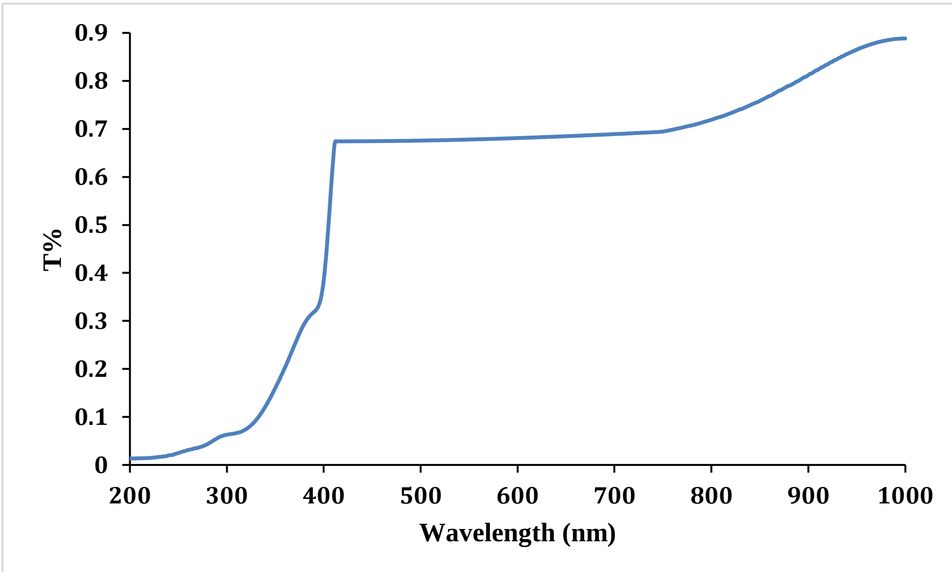


Figure 8: The transmission spectrum of PbI2 films deposited on glass substrate by thermal evaporation

Tauc plot was used to analyze the optical band gap. Figure 9 depicts a linear relationship between $(\alpha hv)^2$ and photon energy. This behavior indicates that a direct permitted transition is possible in the PbI2 film. From the linear part of the curve to the photon energy axis, the optical band gap can be extracted [15]. For PbI_2 thin film, the extrapolation yielded a band gap of 2.65 eV. The energy gap was calculated by using Eq. (2):

$$(\alpha hv)^2 = B(hv - E_g)^n \qquad (2)$$

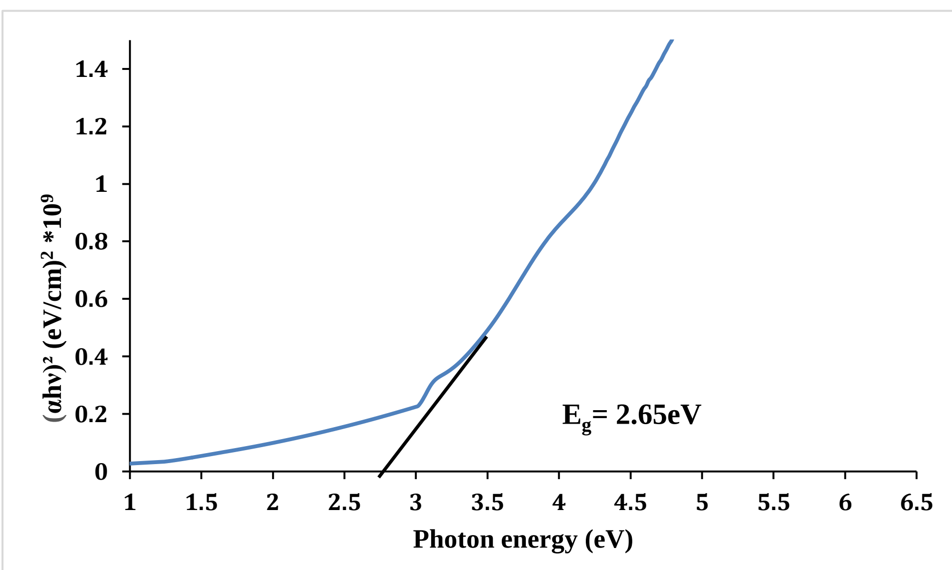
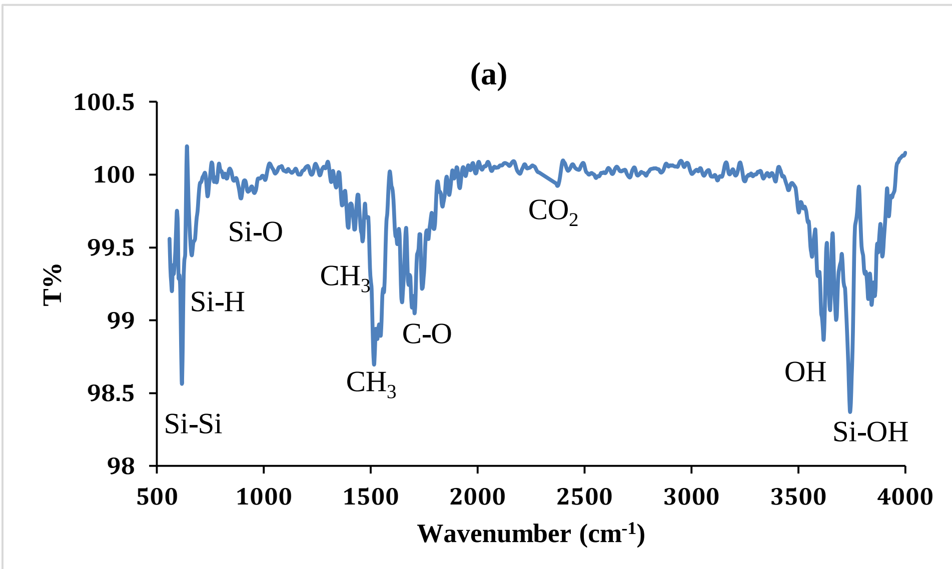


Figure 9: $(\alpha h\upsilon)^2$ vs. $(h\upsilon)$ plot for PbI_2 thinfilm.

FTIR technique is a potent tool for determining the chemical species present in the substance. This approach measures how much radiation can be absorbed by chemical bonds in the substance as the wavelength of the radiation changes in the infrared range. Different chemical bonds absorb different frequencies of radiation [22]. The best way to determine the chemical composition of the PSi surface is to use Fourier Transform Infrared (FTIR) spectroscopy. Because PSi has a substantially bigger specific area than bulk Si, the FTIR signal is larger and easier. The surface of the manufactured PSi layer oxidizes spontaneously after a few hours in ambient air [23]. For original impurities such as hydrogen and fluorine, which are residuals from the electrolyte, the pore surface has a high density of dangling Si bonds. Figure10a shows that the FTIR spectra can be measured from samples at current density (14 mA/cm^2), and etching time (8) minutes. The peaks at around 617 cm-1, 663 cm-1, and 891 cm^{-1} are from Si–Si, Si-H, and Si-O, respectively. The transmittance peak at 1423-1465 cm^{-1} and 1519 cm^{-1}isdue to C-H. The peak at 1708 and 2380 $cm^{-1}$is due to C-O, and peaks at 3614 and 3745 cm^{-1} are due to O-H and Si-OH [24-28]. Figure 10b shows IR spectra of the PbI2 sample that was deposited on the PSi substrate. The peak at frequency 1627 is referred to as the band Pb-I [29]. The peaks around 3412 and 3383cm-1 are due to asymmetric and symmetric stretching vibrations of the Pb–I cluster [30]. It can be noted that the appearance of weak peaks of PbI_2, which perhaps can be attributed to the PSi substrate.



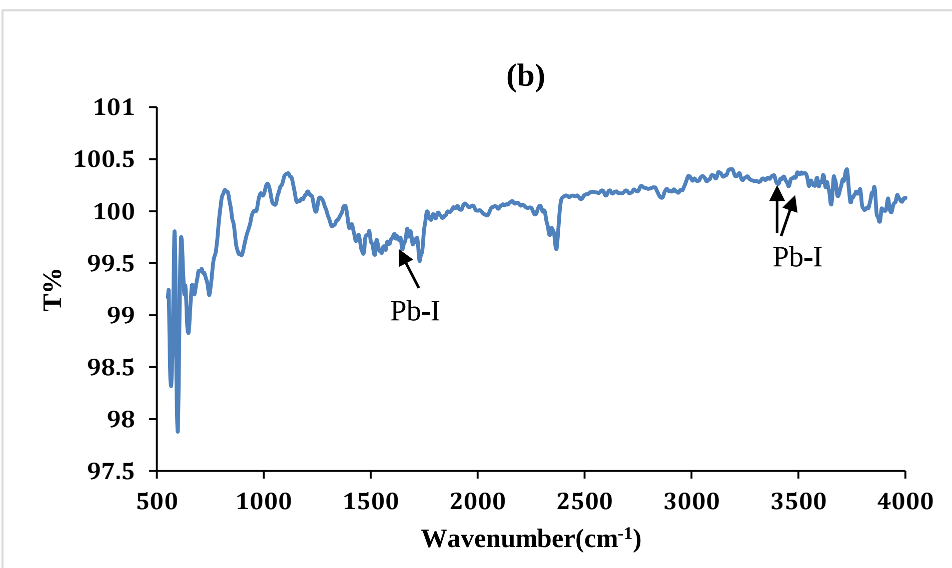


Figure10: FTIR spectra (a): n-PSi layer and (b) PbI_2/PSi Heterojunction.

4. Conclusions

We have prepared and characterized the nanocrystalline porous silicon layer and PbI2 thin film by thermal evaporation technique to study some of its properties. X-ray diffraction showed that the PbI2 film has a hexagonal polycrystalline structure. The band gap energy for PbI2 was estimated to be 2.6 eV. FE-SEM images showed porous silicone via using the photoelectrochemical etching method, the pore distribution is irregular. SEM images of PbI2 film revealed that particles were scattered and resembled gravel in size. The results indicated that PbI2 can be used in physical applications such as solar cells.

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Conflicts of Interest

There are no conflicts of interest.

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