Preparation of Bismuth Oxide Nanoparticles /PSi/Si heterojunction by simple chemical method for solar cell applications

S A Abdullah¹, M H Jaduaa² and A N Abd³*
¹,² Department of Physics, College of Science, Wasit University, Iraq.
²Department of Physics, College of Science, Mustansiriyah University, Iraq.
³Corresponding: ahmed_naji_abdr@uomustansiriyah.edu.iq

Abstract: This work shows the fabrication of Bi₂O₃/PSi heterojunction for solar cell applications prepared by simple chemical method. Bi₂O₃ nanoparticles were deposited on the n-type porous silicon and glass substrates by drop casting method. The structural and optical properties of bismuth oxide thin film were studied by XRD, SEM, UV-VIS and FTIR analysis. XRD investigation showed that the thin film is polycrystalline and the optical properties stated that bismuth oxide thin film has direct optical band gap of 2.5 eV in addition to the study of I-V in dark and under illumination and finally. The results indicate a significant improvement in the properties of porous silicon, and thus an increase in the conversion efficiency, as the calculated efficiency values for (Al/ Bi₂O₃/PSi/Si/Ag) heterojunction.

Keywords: Bismuth oxide nanoparticles, Thin films, structural and Optical properties, Solar cell

1. Introduction

Bismuth oxide thin films have wide attention due to their values of important characteristics parameters such as the energy gap, refractive index, photoconductivity and mechanical strength [1-5]. These films were suitable for many applications such as solar cell, photo detectors, sensor fuel cells, optoelectronic devices[6-8]. Bismuth oxide thin films were prepared by many techniques; simple chemical method, sol-gel, spray pyrolysis, sputtering thermal evaporation and pulsed laser deposition[9-12]. Bi₂O₃ shows a distinctive polymorphism including α-Bi₂O₃, β-Bi₂O₃, γ-Bi₂O₃, δ-Bi₂O₃[13]. In this paper Bismuth oxide solution nanoparticles was prepared by simple chemical method which is one of the simplest methods where nanoparticles can be prepared with very perfect crystallinity and deposited on glass and porous substrates to produce thin films. The structural and optical properties of thin films were investigated.

2. Experimental Work

About 9.87 g of Bi(NO₃)₂ were dissolved in 50 ml of polyvinylpyrrolidone and 100 ml distilled water to give a yellow solution. About 100 ml of 1M NaOH solution was rapidly added to the solution in around flask with Stirring, in this time nanoparticle suspension was formed. The suspension was maintained for one hour at 80°C. After cooling to room temperature, nanoparticles were separated by centrifugation then
washed by distilled water to get rid of pollution, the solution was yellow as shown in Figure (1). After that the solution was taken by pipette, then dropped onto glass porous substrates (4 drops) then the samples were dried at 80°C. The thickness of the thin film was 150 nm which was calculated by the gravitational method. Crystalline wafer of n-type silicon of (2-20)Ω.cm resistivity, 580 μm thickness and (100) orientation were used to form porous (Psi) by using photoelectrochemical etching (PEC) which was achieved in (1:1) (47% HF)-Ethanol and (99.99) mixture at 20°C temperature and (Au) electrode was used in this process as shown in Figure (2).

3. Results and Discussions
The investigations of Bi$_2$O$_3$ thin film structure were achieved by XRD, SEM, AFM and FTIR experimental techniques. XRD investigation shows the structure of Bi$_2$O$_3$ thin film was polycrystalline and multiphase as shown in Figure (3). And the crystalline structure of bismuth oxide thin film was
strongly depend on the process of nucleation and growth for the particles on the substrate of the thin film [6].

![Figure 3. XRD pattern of Bi₂O₃ thin film which prepared by simple chemical method and deposited by drop casting technique on glass substrate.](image)

XRD investigation gives a scientific sight about the nature of the structure of thin film. The XRD for the high ready film shows a peak of Bismuth oxide at 30.25(2θ),32.72(110), 39.49(114), 42.26(114), where corresponding d-values compared with the standard (JCPDS file No:00-050-1088) for Bi₂O₃ as shown in the table (1), and another informations as average size of crystallites (Dav), micro strains (γ), Dislocation Density (δ) were show in table 2.

**Table 1.** values of Inter planer Spacing for Bi₂O₃ compared with d-values in Standard (JCPDS file No:00-050-1088)

| Heat Treatments°C | 2θ (deg) JCPDS | 2θ (deg) Observed | (d) values(Å) JCPDS | (d) Values (Å) Observed | (hkl) Planes |
|-------------------|----------------|-------------------|---------------------|------------------------|--------------|
| 200               |                |                   |                     |                        |              |
|                   | 25.54          | 25.58             | 3.4840              | 3.4848                 | (Bi₆O₆) (102) |
|                   | 31.3           | 31.04             | 2.855               | 2.85                   | (Bi₂O₂) (104) |
|                   | 34.83          | 34.84             | 2.574               | 2.573                  | Bi₆O₆(112)   |
|                   | 39.4           | 39.38             | 2.285               | 2.286                  | Bi₂O₃(114)   |
|                   | 46.2           | 46.18             | 1.962               | 1.964                  | (Bi₆O₆) (116) |
|                   | 47.62          | 47.6              | 1.908               | 1.908                  | (Bi₂O₂) (200) |
|                   | 54.82          | 54.78             | 1.673               | 1.674                  | Bi₂O₂ (212)  |
|                   | 58.11          | 58.08             | 1.5860              | 1.5868                 | Bi₂O₂ (214)  |
Table 2. Lattice Constant (a), Dav, δ, γ, N (Number of Crystallites per unit Area).

| Heat Treatments °C | 2θ (deg) | d (Å) | a (Å) | hkl planes | β (deg) | Dav (nm) | δ×10^{14} (m^{-2}) | γ×10^{-4} | N×10^{15} (m^{-2}) |
|-------------------|---------|-------|-------|------------|---------|---------|-------------------|---------|-------------------|
| 200               | 25.58   | 3.484 | 7.79  | Bi\textsubscript{6}O\textsubscript{6} (102) | 0.294   | 28.06   | 1.27              | 1.28    | 6.789             |
|                   | 31.04   | 2.855 | 11.77 | Bi\textsubscript{6}O\textsubscript{6} (104) | 0.334   | 24.70   | 1.73              | 1.46    | 9.95              |
|                   | 34.83   | 2.57  | 6.30  | Bi\textsubscript{6}O\textsubscript{6} (112) | 0.304   | 27.14   | 1.35              | 1.33    | 7.50              |
|                   | 39.39   | 2.28  | 9.69  | Bi\textsubscript{6}O\textsubscript{6} (114) | 0.393   | 20.99   | 2.26              | 1.72    | 1.62              |
|                   | 46.18   | 1.964 | 12.1  | Bi\textsubscript{6}O\textsubscript{6} (116) | 0.368   | 22.42   | 1.98              | 1.6     | 1.33              |
|                   | 47.62   | 1.908 | 3.8   | Bi\textsubscript{6}O\textsubscript{6} (200) | 0.266   | 31.02   | 1.03              | 1.16    | 5.02              |
|                   | 54.78   | 1.67  | 5.01  | Bi\textsubscript{6}O\textsubscript{6} (212) | 0.376   | 21.94   | 2.07              | 1.64    | 1.42              |
|                   | 58.08   | 1.586 | 7.26  | Bi\textsubscript{6}O\textsubscript{6} (214) | 0.44    | 18.7    | 2.85              | 1.92    | 1.70              |

AFM image is shown in figure (2) states that the morphology of the surface was simply like the agglomerated fibers groups and this was caused by attraction force between any two different particles in charge in addition to the nano size of particle makes it surrounding by charges so the structure of thin film becomes polycrystalline and according to AFM it seems semi homogeneous.

Figure 4. AFM image of Bi2O3 thin film.
From AFM investigation, the average diameter size is (96.49 nm) and roughness average (8.27 nm), as shown in Table 3.

**Table 3.** Roughness, Average Diameter Size and Root mean Square for Bismuth Oxide Nanoparticles thin films.

| Heat Treatments°C | Average Diameter Size (nm) | Roughness Average (nm) | Root Mean Square (nm) |
|-------------------|-----------------------------|------------------------|----------------------|
| 200               | 69.49                       | 8.27                   | 9.55                 |

SEM investigation proves that the surface of bismuth oxide thin film consist of many fibers with the average particle size about 30 nm.

![SEM image of Bi₂O₃ thin film](image)

**Figure 3.** SEM image of Bi₂O₃ thin film prepared by simple chemical method. The grain size was about (24.7-42.34) nm.

FTIR for Bi₂O₃ proves the existence of bismuth oxide in the structure of thin film as shown in figure(4). The bonds which were found in the structure were tabled in Table 4.
Figure 6. FTIR for bismuth oxide thin film.

Table 4. FTIR Assignments for Bi$_2$O$_3$

| Wavenumber(cm$^{-1}$) | FTIR Assignment |
|-----------------------|-----------------|
| 840                   | Bi-O            |
| 1369.5                | C-H             |
| 1633.7                | C-N             |
| 1732.13               | C-O             |
| 2400                  | N-H             |
| 2355,126              | C≡C             |
| 3288.7                | O-H             |

Figure (5) represent the optical absorption spectra in 300-900 nm spectral range proving the good transmittance in the visible region.
Figure 5. Optical absorption spectrum of bismuth oxide thin film.

The energy gap was calculated using the equation:

\[(\alpha h\nu)^2 = A(h\nu - E_g)^n \] (1)

Where \(\alpha\) is the refractive index, \(h\nu\) is the energy gap of the incident photon, \(A\) is a band edge parameter and \(n\) is the refractive index. \(E_g\) was calculated by extrapolating the straight line portion \((h\nu\alpha)^2 = 0\) the result of the energy gap is about \((0.45\ \text{eV})\) as shown in figure(6)[14].

Figure 6. \((\alpha h\nu)^2\) versus photon energy gap of Bi₂O₃ thin film.
4 -Dark I-V measurements

Solar cell convert light to electricity illumination conditions, small in fluctuations of the intensity of light introduces significant amount of noise to the system making it hard to produce accurate readings. Dark I V measurements inject carriers into the circuit with electrical methods rather than light generated carriers [15]. It providing an effective way to determine the formations about short –circuit current, series resistance and shunt resistance[ 6]. the figure (7) shows the dark I-V properties of (Al/Bi2O3/PS/Si/Ag).

Figure 7. Dark I-V characteristics of (Al/Bi2O3/PS/Si/Ag).

I-V characteristics under illumination it can be seen from the figure (8) where the current value at a given voltage for(Al/Bi2O3/PS/Si/Ag) is higher than that in dark this was happened because of the production of electron–hole as a result of the light absorption[16].
Figure 8. dark and illuminated (I-V) characteristics of (Al/Bi2O3/PS/Si/Ag).

The characteristic of (I-V) for solar cell (Al/Bi2O3/PS/Si/Ag) is shown in figure(9).

![I-V Characteristics](image)

Figure 9. The characteristics of solar cell (Al/Bi2O3/PS/Si/Ag).

According to figure(9) the value of fill factor is (31.6) and finally the efficiency of the solar cell is (6.8) where the incident power is $\frac{40\text{mW}}{cm^2}$ AS in Table 5.

| Heat Treatments | Parameters |
|-----------------|------------|
| Si Type | Voc (volt) | Isc (mA) | $V_{\text{max}}$ (volt) | $I_{\text{max}}$ (mA) | Fill Factor(FF%) | Efficiency (\(\eta\)) |
| 200°C | n-type | 4.1 | 1.45 | 2.4 | 0.89 | 36.2 | 6.8 |
5. Conclusions:
The prepared Bi2O3 is in nanosized by simple chemical method. The stricter of thin film was polycrystalline with roughness about (8.7nm) The absorption of the structure increases with wavelength. Energy gap for Bi2O3 was (2.45eV) The current at a given value of voltage under illumination was higher than that in dark. efficiency of solar cell (Al/Bi2O3/Psi/Si/Ag) was 6.8.

6. REFERENCES
[1] H. Gobrecht, S. Seeck, H. Bergt, A. Martens, K. Kossmann, Phys. Stat. Sol. vol. 33, pp.599, 1969.
[2] V. Dolocan, F. Iova, Phys. Stat. Sol., vol. A64, pp.755, 1981.
[3] P. Clapham, J. Appl. Phys., vol.18, pp.363, 1967.
[4] T. Nikolov, M. Avoyo, E. Klein, K. Ikonopisov, Thin Solid Films, vol.30, pp.37, 1975.
[5] L. Leontie, M. Caraman, M. Alexe, C. Harnagea, “Structural and optical characteristics of bismuth oxide thin films,” Surface Sciences, vol. 507 – 510, pp.480-485, 2002.
[6] S. Arya, H. Singh, Thin Solid Films, vol.62, pp.353,1979.
[7] G. Bandoli, D. Barecca, E. Brescacin, G. Rizzi, E. Tondello, Chem. Vap. Depos., Vol. 219, pp.238,1996.

[8] T. Hyodo, E. Kanazawa, Y. Taka, Y. Shimizu, M. Egashira, Electrochemistry, Vol. 68, pp. 24, 2000.
[9] Rahi, S.K., Nasser, Z.S., Shakir, I.A. The effect of gamma rays in some optical and physical properties of the material (PVA) dissolved in distilled water, Journal of Global Pharma Technology, 2019, 11(2), pp. 593–600
[10] Abd, A.N., Abdullah, M.T., Rahi, S.K., Habubi, N.F., CdO/FTO Schottky photodetector with enhanced spectral responsivity and Specific detectivity prepared by electrolysis method Journal of Physics: Conference Series, 2020, 1660(1).
[11] L. Leontie, M. Caraman, M. Delibas, G. Rusu, “Optical properties of bismuth trioxide thin films,” Materials Research Bulletin, vol.36, pp.1629-1637, 2001.
[12] Nadir F. Habubi1, Raid A. Ismail, Ahmed N. Abd (2014); Synthesis and characterization of nano crystalline porous silicon layer for solar cells applications.
[13] R. Ismail, O. Abdulrazzaq, “Preparation and photovoltaic properties of Ag2O3/Si isotype heterojunction,” Surface Review and Letters, vol.12, no.2, pp.299-303, 2005.
[14] HABUBI, N.F., ABD, A.N., DAWOOD, M.O., and RESHAK, A.H. (2018) Fabrication and Characterization of a p-AgO/PSi/n-Si Heterojunction for Solar Cell Applications. Silicon, 10 (2), pp. 371-376.
[15] HABUBI, N.F., HASSONI, M.H., ASIS, W.J., and ABD, A.N. (2019) Invention and Description of p-CuO /n-Si (200 oC) Heterojunction for Photodiode Applications. Journal of Global Pharma Technology, 11 (2), pp. 601-606.
[16] [33] Abd, A.N., HABUBI, N.F., RESHAK, A.H., and MANSOUR, H.L. (2018) Enhancing the Electrical Properties of Porous Silicon Photodetector by Depositing MWCNTs. International Journal of Nanoelectronics & Materials, 11 (3), pp. 241-248.