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Structural and Optical Properties for TiO_2 thin films Prepared by Screen Printing method

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ABSTRACT

In this study, Structural and Optical Properties of titanium dioxide thin films are studied, TiO_2 (Anatase) thin films were prepared by screen printing (SP) method. X-ray diffraction analysis showed that the structure of TiO_2 films are polycrystalline and the lattice system is tetragonal. The main diffraction peak of TiO_2 was (101) at $2\theta=25^{\circ}$. The data of optical absorption indicated that TiO_2 thin films prepared by SP have a direct optical band gap (about 3.1eV). The data of reflectivity was also used to calculate the band gap and was around 2.95 eV

Introduction

TiO_2 is semiconductor metal Oxide that has unique properties such as low cost, nanotoxicity, easy reation and resistance to chemical corrosion. It is used in environmental purification applications as well as in the manufacture of solar cells and other applications such as anti-moisture lenses, photoelectrochemistry, electro chromic devices, catalysis, gas sensing and dye-sensitized solar cells [1]. TiO_2 material to be much impartant than any thing else, because of the ability to work as a photovoltaic catalyst whose most important condition is to generate an electron pair- a gap near the surface of the catalyst by shedding a large part of the solar spectrum [2,3]. Titanium dioxed (TiO_2) was first produced commercially in 1923. Titanium dioxed is obtained from avariety of Ores, TiO_2 exists mostly as Rutile and Anatase phases which both of them have the tetragonal structures rutile is high-temperature stable phase and has an optical energy band gap of 3.0eV (415nm), Anatase is formed at a lower temperature with an optical energy band gap of 3.2eV and refractive index of around 2[4]. There are many processing techniques that can be used to prepare TiO_2 thin films such as Sol-gel, Liquid deposition, electron-beam, evaporation, chemical vapour deposition (CVD), direct current (DC), radio frequency (RF), plasma oxidation, magnetron sputtering [5], we used new method which is screen printing processes for thin films preparation where they are widly applied because of their uniformity and rapid production as well as easy thickness control [6]. this study showed the feasibility to fabricate TiO_2 electrodes from dioxide nano-powder, terpineol, ethanol and ethyl cellulose to be used in dye sensitized solar cell using screen printing method which is simple and low cost technique.

Experimental details

For making the paste, the following materials were used: titanium dioxide TiO_2 (purity 99.9%) of mass 0.34g, Ethanol volume 3ml, Terpineol 2ml and Ethyl cellulose of mass 0.032g as a binder. Glass slides were used as substrates for TiO_2 thin films, The substrates were cleaned with ethanol solution and distilled water, Then they immersed for 30 min in distilled water then dried with special drying paper and we used Scotch tape for framing. The past is prepared in the clean room and take some drop of past to deposited on the glass and quartz. All the samples were annealed in furnace at 500℃ for 30 minutes and then left in the oven overnight to cool down. XRD measurements were implemented using Shimadzu XRD model-6000. The absorption spectra were measured Via a spectrophotometer provides (Meterteach Sp 8001) at room temperature and Tauc plot was utilized to calculate the band gap, The film thickness was calculated using the micrometer where it measures the first reading without paste and the second reading with the paste, the difference between them is the thickness of the film thin, The Atomic Force Microscope (AFM) has been used and provides information on the nanoscale structure of the thin films and gives 2D and 3D analysis of the surfaces of the studied thin films,type AA3000-The provider from company Angstrom Advanced, device specifications: X-Yscan Scope:~10 micrometer, 2 distance:~ 2 micrometer, Scan Angle: 0-360 degree, Scan Rate: 0.1~ 100HZ, Size=2032×2044nm.

Results and Discussion

X-Ray Diffraction

Figure (1) shows XRD patterns of TiO_2 thin films prepared by screen printing method, intensity of diffraction X-ray was recorded for range 2θ from 10^o to 80^o. The main diffraction peaks of TiO_2 thin film after annealing at 500^oC were (101) at $2\theta = 25^\circ$, and the phase of TiO_2 is Anatase, this result agrees with findings referenc [7, 8], as well as it is seen that full width half of maximum (FWHM) values were listed in Table (1) The grain size (D) of the films was calculated from the FWHM values using the Debye-Scherer's formula[9] :

$$D = \frac{0.9\lambda}{\beta \cos\theta} \quad .....(1)$$

Where D is the crystal size ; λ the X-ray wavelength (λ=0.15406 nm), K is usually taken as 0.9 , β is the line width at half-maximum height in (radian) , and θ is the Bragg diffraction angle.

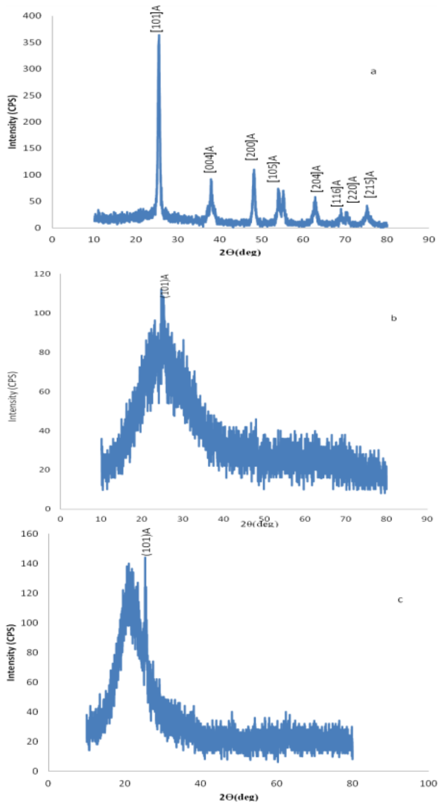

Figure (1): XRD pattern TiO_2 (a) powder of TiO_2 nanopaticles (b) TiO_2 thin film on quartz (c) TiO_2 thin films on glass

Scherrer analysis for TiO_2 powder is indicated in Table (1). The average crystallite size is about 16.3 nm while the average line density is 0.0038 lines/nm^2.

Table (1): Scherer's analysis of TiO_2 nanopowder

2θ(deg)	D (nm)	S(lines/nm^2)	FWMH (rad)
25.4	17.05	0.0039	0.0083
37.84	17.1	0.0034	0.0091
48.16	16.0	0.0039	0.0096
53.9	15.7	0.0040	0.0094
55.18	15.7	0.0040	0.0096
62.8	16.5	0.0036	0.0098

Williamson and Hall proposed [6] a method for determination size and strain broadening by looking at the peak width as a function of 2θ. According to this analysis, the total broadening (B_{tot}) in each peak is produced by two

types of broadening, strain broadening (β_{strain}) and size broadening (β_{size}) i.e.

$$\beta_{tot} = \beta_{strain} + \beta_{size} \quad .....(2)$$

Where $\beta_{strain} = 2\varepsilon \tan\theta$ and $\beta_{size} = \lambda / D\cos\theta$.

After some simple algebra we can rewrite (2) as follows:

$$\beta^* = \varepsilon d^* + \frac{1}{D} \quad ......(3)$$

Where $\beta^* = \beta\cos\theta/\lambda$ and $d^* = 2\sin\theta/\lambda$. (Williamson-Hall) plot is shown in fig (2) It is plotted with $\beta\cos\theta$/λ on the y-axis and $2\sin\theta$/λ on the x-axis. A linear fit is got for the data and from it: particle size (20 nm) and strain (0.00006) are extracted from y-intercept and slope – respectively.

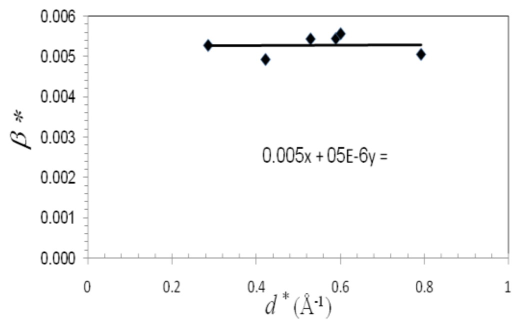

Fig (2) Williamson-Hall plot-TiO_2 nanoparticles

Atomic Force Microscopy (AFM)

The surface Topology of TiO_2 thin films was analyzed using atomic force microscope. Figure (3) represents the result of AFM scanning in three dimensions for TiO_2 paste deposited on glass slides by SP and fired at (T=500) °C. The two diagrams show the typical three-dimensional surface Topology image of TiO_2 and the granularity distribution, respectively. The average grains size for TiO_2 films after annealing 500 °C for 30 min.) is about 57 nm and the roughness average is roughly 3 nm, root mean square was about 3.4 nm. The shape of the thin film is regular and homogeneous, and the adhesion strength was very good through these tests where the arrangement and uniformity of the coating layers are clear, and it is important to observe that notice that the particles are vertically perpendicular to the crystal axis.

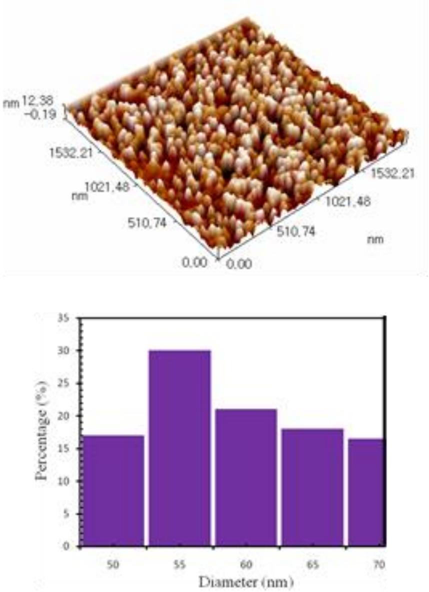

Fig (3) (a) AFM image for TiO2. (b) The granularity cumulation distribution chart of TiO_2 thin films

Optical Properties

The transmission spectrum of TiO_2 thin films is recorded as a function of wavelength in the range of (190-990) nm as shown in Figure (4). The thickness of TiO_2 was too thin (about 500 nm) for TiO_2 deposited on glass and quartz substrates so that the average transmission over the visible rang could exceed 20 %.

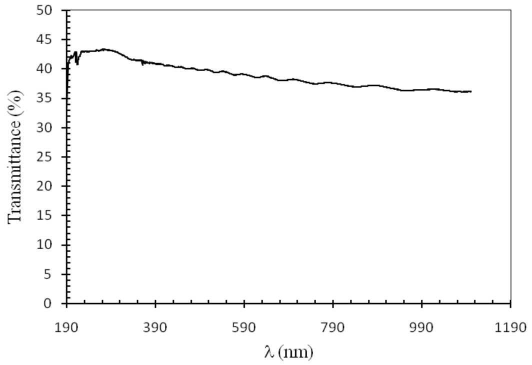

Fig (4):Transmittance spectrum of TiO_2 prepared by screen printing

The optical bandgap (E_g) has been analyzed using Tauc plot [10] in which the relationship between absorption coefficient (α) and photon energy $(h\nu)$ is given by:

$$\alpha h\nu = B(h\nu - E_g)^n \quad \ldots(4)$$

Where B : constant depends on the type of transition.
hν: photon energy.
E_g: direct allowed energy photon.
n: exponential constant. n=1/2 for TiO_2

The absorption (α) was determined from the absorbance spectrum using the following equation [11]:

$$\alpha = 2.303\frac{A}{t} \quad \ldots(5)$$

Where A is the measured absorbance and t is the thickness of the sample. Fig (5) shows the relation of $(\alpha h\nu)^2$ against photon energy, from strainst line obtained at high photon energy the direct allowed energy gap could be determined, The optical band gap energy E_g was evaluated from the absorption spectrum and the optical absorption coefficient (α) near the absorption edge is given by Eq (4), The extrapolation gave a bandgap of 3.1eV for our TiO_2 thin film prepared by SP. This result has a good a agreement with the findings reference[12].

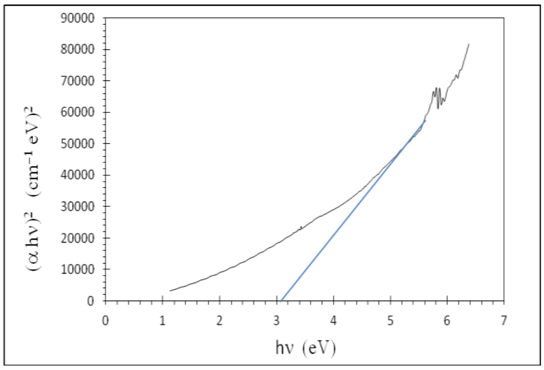

Fig. (5): plot of $(\alpha h\nu)2$ versus hν of TiO_2 thin film

Diffusive reflectance spectra

Diffusive reflectance spectra can also be used to calculate the absorption edge of TiO_2 [11]. Figure (6) shows the reflectance which is plotted as a function of photon energy in the range from (1.5-4.0) eV for TiO_2 thin films deposited on glass substrates by screen printing technique. The sharp full of reflectance determines where the sample starts to absorb near the band edge. The intersection point between the extrapolation line and the hν-axis gives the value of energy band gap (E_g) the results obtained for the band gap are in good agreement with results extracted from Tauc plot.

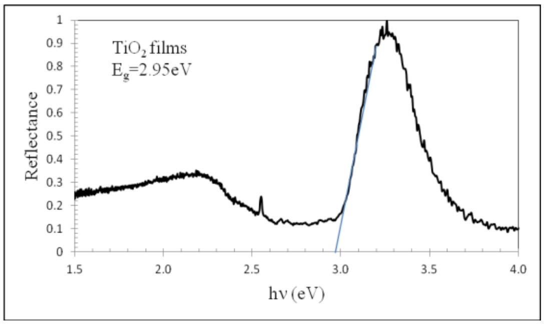

Fig (6) Determination the energy band gap of TiO_2 thin films using diffusive reflectance data.

Conclusions

Synthesis of TiO_2 thin films by screen printing method is found to be fast, low cost and practical to prepare electrodes dye sensitized solar cells. TiO_2 thin film prepared by screen printing method and fried at500°C is polycrystalline with a broad peak located roughly at $2\theta = 25^{\circ}$. The grain size increased after annealing (500 °C for 30 min.) to become 57 nm. The band gap of TiO_2 thin film is direct with energy bandgap of 3.1 eV. Diffusive reflectance method gives accurate value for bandgap energy and compatible with that calculated from Tauc plot.

References

[1] Kavitha, Mrs. M.; Gopinathan, Dr. C. and Pandi, P. P. (2013). Synthesis and characterization of TiO_2 Nanopowders in Hydrothermal and Sol-Gel Method. *International Journal of Advancements in Research and Technology*, **2(4)**: 102-108.

[2] Sanchez, C.V. H.; Enrique, C. and Lopez, Y.C.M. (2014). Quantification of phase content in TiO_2 thin films by Raman spectroscopy. *Superficies Y Vacio*, **27**: 1665-3521 .

[3] Mugundan, S.et al. (2015). Synthesis and Characterization of undoped and cobalt-doped TiO_2 nanoparticles via Sol-gel technique. *Applied Nanoscience*, **5**: 449-456.

[4] Comert, B.; Akin, N.; Donmez, M.; Saglam, S and Ozcelik, S. (2016). Titanium Dioxide thin films as methane Gas sensors. *IEEE Sensors Journal*, **16 (24)**:1558-1748.

[5] Abdel-Galil, A.; Ali, H. E and Balboul, M.R. (2014). Influence of nanostructured TiO_2 additives on some physical characteristics of Carboxymethyl cellulose(CMC). Journal *of Radiation Research and Applied Sciences*, **7**: 36-43.

[6] Williamson, G. K. and Hall, G. K. (1953). X-ray Broadening from field Aluminium and Wolfram . *Acata Metallurgica*, **1**: 22-31.

[7] Chu, L. Q, Z.; Yang, J. P. and Li, X. (2015). Anatase TiO_2 Nanoparticles with exposed {001} facets for efficient Dye-Sensitized solar cells. *Scientific Reports*, **5**:1-10.

[8] Chengtu, Ch.; Huang, Y. S.; Huang, J. W.; Chang, Ch. K and Wu, Sh. P. (2010). Amacroporous TiO_2 Oxygen Sensor for bricated using Anodic Aluminium Oxide as an etching mask . *Sensors*, **10**:670-683.

[9] Thagarelu, K.; Annamalai, R and Arulndhi, D. (2013). Preparation and Characterization of Nanosized TiO_2 power by Sol-Gel precipition Ronte. *International Journal of Emerging Technology and Adranced Engineering*, **3(1)**: 636-639.

[10] Tauc, J.; Grigorovici, R and Vancu, A. (1966). Optical properties and electronic structure of amorphous germanium. *Physica Status Solidi*, **15**: 627–637.

[11] Mohan, R.; Drbohlavova, J. and Hubalek, J. (2013). Water - dispersible TiO_2 nanoparticles Via a biphasic Solvothermal reaction method. *Nanoscale Research letters*, **8:503**: 1-4.

[12] Saleh, A. F.; Jaffar,A. M.; Samoom, N. A . and Mohmmod, M.W. (2014). Effect Adding PVA Polymer on Structural and optical proportion of TiO_2 thin films. *Journal of Al-Nahrain University*, **17(2)**: 116-121.

[13] Ayieko, C.O.; Musembi, R. J.; Waita, S. M.; Aduda, B.O and Jain, P.K. (2012). Structural and Optical Characterization of Nitrogen-doped TiO_2 thin films Deposited by spray Pyrolysis on Fluorine Doped Tin Oxide (FTO) Coated Glass Slides. *International Journal of Engineering*, **2(3)**:76-72.

الخصائص التركيبية والبصرية للأغشية TiO_2 المحضرة بطريقة طباعة الشاشة

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الملخص

في هذا العمل, تم دراسة الخصائص التركيبية والبصرية لأغشية ثنائي أوكسيد التيتانيوم, وتبين أن أغشية TiO_2 التي تم تحضيرها بطريقة طباعة الشاشة (SP). تظهر أن تحليل حيود الأشعة السينية بأن تركيب أغشية TiO_2 متعدد التبلور ونظام الشبكة هو رباعي الأضلاع , وأن قمة الحيود الرئيسية لأغشية TiO_2 كانت (101) عند $2\theta=25^{\circ}$, بيانات الإمتصاص البصري أشارت بأن أغشية TiO_2 المحضرة بطريقة طباعة الشاشة تمتلك فجوة طاقة بصرية مباشرة حوالي (3.1eV), تم حساب قيم فجوة الطاقة بواسطة نتائج قيم الإنعكاسية وكانت (2.95eV).