IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 8, Issue 6 Ver. V (Nov. - Dec. 2016), PP 10-13
www.iosrjournals.org

Using mathematical methods to calculate some optical properties of Titanium DioxideTiO_2

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***Abstract**: This paper examines Optical property of Titanium Dioxide TiO2.there for we have after practical on the samples we find all The samples showed high transmission in the UV region with transmission edges in the blue region of the electromagnetic spectrum. also we had been found rapidly decrease in absorption coefficient value , until to arrive to peak, then it reduce from high temperature because of less absorption in high energies from energy gap Transition decreasing due to transmission decreasing.*
***Keywords:** TiO2, The optical band gap, Optical property.*

I. Introduction

In this work, we study of the optical properties of Titanium dioxide. We study the relation between wavelength and absorption and transition and wavelength. There are many applications and uses of Titanium dioxide. For example, the white titanium used in color [11] and coloring and is a metal with a gray color found in the Earth's skin general in layers since formed the earth as there is in the air and water at different rates in addition to the occurrence in plants that nurtured them. Also it used as a color. There for that are much kind of applications of Titanium dioxide, like from paint to sunscreen to food coloring [6].TiO_2 Nanoparticles usually used in suntan lotion as part of the creation to block the sun is damaging UV rays. In addition, TiO_2 nanoparticles used in consumer products has increased; concern has risen as to the health and environmental effects of nanoparticles. There for sunscreens contact skin and wash off in water, hence the TiO_2 nanoparticles be able to find their way into biological and environmental systems. Therefore, we need to measure both the size and size scattering of these nanoparticles in sunscreens, then as to calculate their impact on human health and the environment [7,12]. The other application of titanium dioxide areas are paints and varnishes as inks and fibers and rubber also we say it used in other applications, for example the manufacture of technical pure titanium, glass and glass tiles [8] also it used as a new electronic circuit element[9]. Particularly Titanium dioxide, in the anatase form, is a photo catalyst under infrared (UV) light. Moreover, It has been reported that titanium dioxide, when doped with nitrogen ions or doped with metal oxide like tungsten trioxide, is also a photo catalyst under either visible or UV light.[10] And finally can be written many applications and usesof the strong oxidative potential of the positive holes oxidizes water to create hydroxyl radicals. Moreover, it oxidize oxygen directly and its use as a dye, and we can add the titanium dioxide to strengthens and to tiles or other products [13].

II. Experimental Section

Sol Synthesis

Sol was prepared by dissolving tetrabutyltitanate ($Ti(OC_4H_9)_4$, TBOT) and tetraethyl orthosilicate($Si(OC_2H_5)_4$, TEOS) in anhydrous ethanol (C_2H_5OH, E_tOH). Deionized water (H_2O) was used forhydrolysis, with acetyl acetone($CH_3COCH_2COCH_3$, AcAc) as chelating agent and acetic acid($CH\_3\ COOH, HAc$) as catalyst. During the synthesis, two different but equal parts of ethanolicsolutions were prepared. In the first part, TBOT was dissolved in anhydrous ethanol containing$AcAc$.after mixed with HAc, the solution was then sealed and stirred for 30 min to achieve a completechelation between the all oxide and $AcAc$. The second part of the solution was then prepared bymixing the TEOS and demonized water with anhydrous ethanol. These two solutions were then mixedand stirred for 2 h to achieve hydrolysis and condensation. The molar ratio wasTBOT: TEOS: E_tOH: H_2O: HAc: AcAc = 1:1:30:5:2:1. The mixture was finally aged in a stableenvironment (with humidity lower than 30% and temperature of 20~25 °C) for 48 h.2.2. CoatingPreparation .The silicon wafer and silica glass substrates were firstly cleaned thoroughly, heated at 200 °C for20 min, and then cooled down to room temperature. A dip-coating apparatus (CHEMAT DipMaster-200) was used for the depositions, and the film thickness could be adjusted by the withdrawplate (0~12 inch/min). After each coating, the films were first pretreated at 100 °C for 1h, and thenheat-treated in a muffle furnace for 2 h at different temperatures ranging (300 -600 and 900 °C). All thecoating processes of the samples were the same to make sure that the properties of the films annealed at different temperatures could be accurately compared and studied.

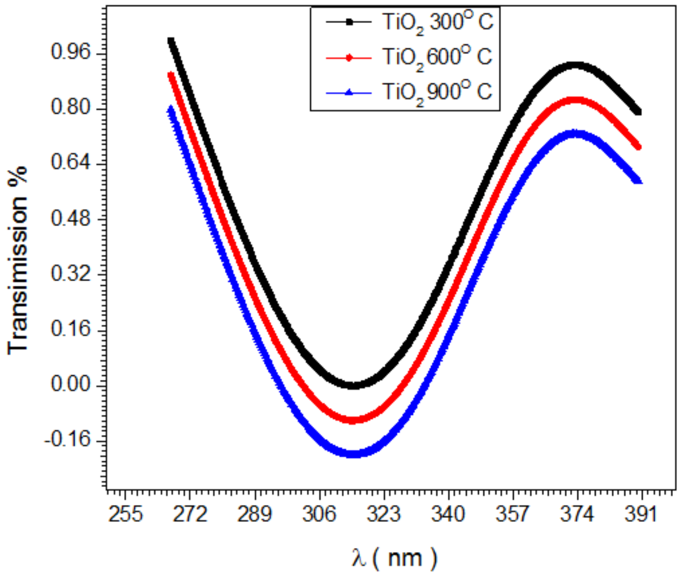

Fig (1)

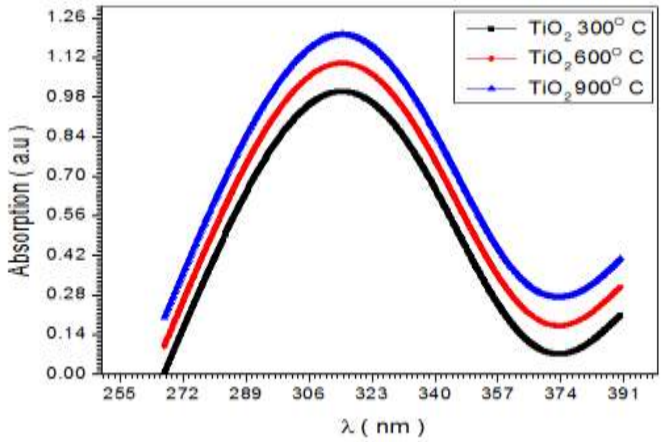

Fig (2)

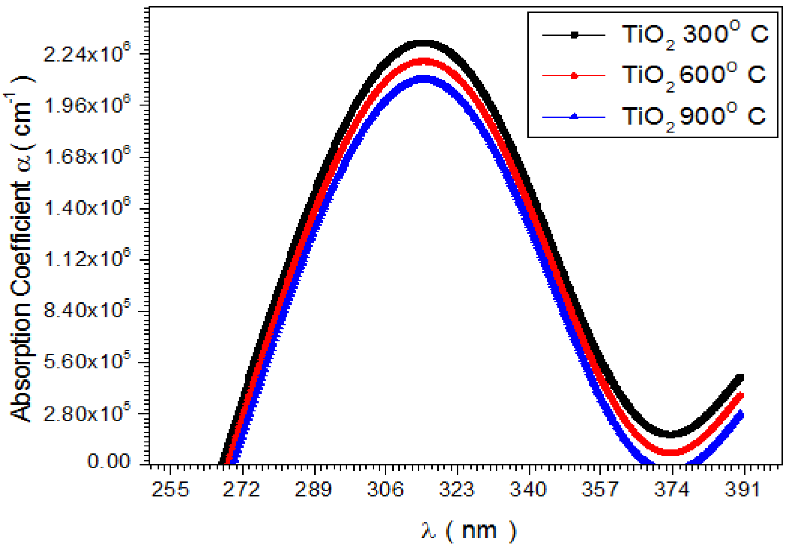

Fig (3)

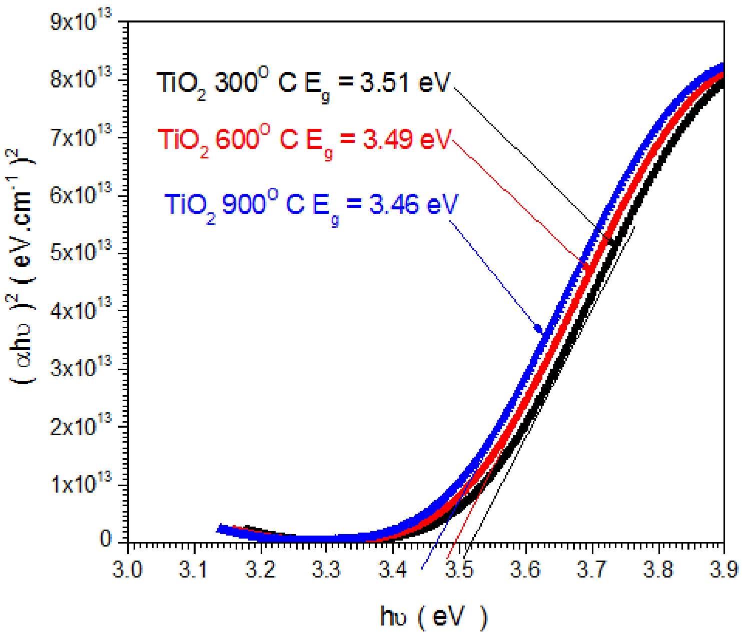

Fig (4)

III. Discussion

In figure (1) shows the transmission plot as a function of wavelengths as obtained from the UV-VIS spectrophotometer. The transmittance and reflectance were calculated using Beer Lamberts and assuming negligible scattering .The samples all showed high transmission in the UV region with transmission edges in the blue region of the electromagnetic spectrum. Photo activation of TiO2 in this region causes transition from the ground to excited state .The electrons transit to the impurities energy level induced by photo catalytic centers TiO2 when being photo activated by blue light ,whichagrees with [2]. This Explains why illumination of TiO2 samples with UV mercury lamp produces fluorescent O2 Nano clusters as some research also assume [3]. There was rapid increase of the absorption in the high temperature. Fig (3) shows the relation between absorption coefficient and wavelengths. we had been found rapidly decrease in absorption coefficient value .until to arrive to peak, then it reduce from high temperature because of less absorption in high energies from energy gap Transition decreasing due to transmission decreasing .At low energies from energy gap, the a absorbance is increasing, this cause the reduce in reflection, and the upper corresponding energy gap value (2.2 - 2.6) eV. And the plots of normalized values of $(\alpha h\nu)$ 2 vs.$h\nu$ are obtained. Sample plots showing the variation of $(\alpha h\nu)$ 2 vs.$h\nu$ obtained from TiO2 are shown in Fig. (4) Respectively as sample results. From such curves, energy band gap of the fabricated films can be evaluated as some research also assume[3, 4, and 5]. The relation between the absorption coefficient (α) and the incident photon energy $h\nu$ is given by,

$$(Ah\nu)^2 = A(h\nu - Eg)$$

Where, A is a constant andE_g is the band gap energy. The optical band gap E_g is determined from the plot of normalized values of $(\alpha h\nu)$2 vs$h\nu$for direct allowed transition, as shown in the samples plots, given in Fig 1. The intercepts of the tangents to the plots, give a good approximation of the band gap energy for direct band gap material [4, 5]. The band-gap of TiO2 samples are found to be 3.51 eV from 300 OC, 3.49 eV from 600 OC and 3.46 eV from 900 OC respectively.

IV. Conclusions

In this paper, we study the UV Visible spectrophotometer we find all the samples showed high transmission in the UV region with transmission edges in the blue region of the electromagnetic spectrum.

References

[1] X. Y. Zhang, X. Y. Pan, Q. F. Zhang et al., "Synthesis of silver oxide nano-scale thin films and photo-activated dynamic luminescence fromtheir nanoparticles," Acta Physico—Chimica Sinica, vol. 19, no. 3, pp. 203–207, 2003.

[2] L. A. Peyser, A. E. Vinson, A. P. Bartko, and R. M. Dickson, "Photoactivated fluorescence from individual silver nanoclusters," Science, vol. 291, no. 5501, pp. 103–106, 2001.

[3] N.R.C.Raju, K. J. Kumar, andA. Subrahmanyam, "Silver oxide (AgO) thin films for surface enhanced Raman scattering (SERS) studies," AIP Conference Proceedings, vol. 1267, pp. 1005–1006, 2010.

[4]. T.K.Subrayman , B.Srinivasulu and S.Utnanna , Cryst.Res. Technol., 35,10,1193(2000).

[5]. N. Benramdane, WA. Murad, RH.Misho, M.Ziane and Z.Kebbab, Materials Chmistry and physics , 48,2,119-123(1997).

[6] "Mineral Commodity Summaries, 2015" . U.S. Geological Survey. U.S. Geological Survey 2015.
[7] Dan, Yongbo et al. Measurement of Titanium Dioxide Nanoparticles in Sunscreen using Single Particle ICP-MS. perkinelmer.com
[8] Emsley, John (2001). Nature's Building Blocks: An A–Z Guide to the Elements. Oxford: Oxford University Press. pp. 451–53. ISBN 0-19-850341-5
[9] Lewis, Nathan. "Nanocrystalline TiO2". Research. California Institute of Technology. Archived from the original on 16 April 2009. Retrieved 9 October2009.
[10] Greenwood, Norman N.; Earnshaw, Alan (1984). Chemistry of the Elements. Oxford: Pergamon Press. pp. 1117–19. ISBN 0-08-022057-6
[11] https://en.wikipedia.org/wiki/Water.
[12] http://health.mo.gov/training/epi/Mod4StudentOutline.
[13] http://www.slideshare.net/shonasrish/advanced-building-materials