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Synthesis and Characterization (Optical, Band Positions and Electrical) of TiO_2 Nano Crystalline

[1]Mubarak Dirar Abd-alla ,[2]Hiba Min Alla Elobeid Gibreel, [3]Abdalskhi .S.M.H & [4]Ahmed Alfaki

[1]Sudan University of Science &Technology-College of Science-Department of Physics & International University of Africa-College of Science-Department of Physics- Khartoum-Sudan
[2-4]Sudan University -Science and Technology Faculty of Science Physics- Khartoum- Sudan
[3]Al-Neenlen University- Faculty of Science and Technology- Physics Department- Khartoum- Sudan

Abstract: *Titanium dioxide (TiO_2), Nano crystalline was synthesized by $TiCl_4$ solution was slowly added, it is distilled water in an ice bath. The Ultraviolet-visible (UV-Vis) spectrometer min 1240 to carry out the optical properties , the maximal optical absorbance value at240 nm corresponding photon energy 5.17 eV ,while absorption coefficient value equal $1.52x10^4$ cm^{-1} at the same wavelength, maximum value of (n) is (2.19) ,optical energy band gap equal (3.773) eV and high magnitude of optical conductivity ($1.17x10^{11}$ sec^{-1}) confirms the presence of very high photo-response .The infrared spectra of Titanium dioxide (TiO_2) was used to locate the band positions, H-O-H bending vibration of free or absorbed water which implies that the hydroxyl groups are retained in sample at 3440 cm^{-1}.*

Keywords: *Titanium Dioxide, Nano crystalline, Optical Properties, Band Positions, Optical Conductivity.*

Introduction

Titanium dioxide is a metal oxide mineral composed of the elements of titanium and oxygen with the chemical formula TiO_2. Titanium dioxide has three crystalline forms including rutile, anatine and brocite. Usually at low temperatures, titanium dioxide crystallizes as anatine phase. With high temperature, the semi-stable phase of anatine transforms into a stable phase of rutile in one transformation [1, 3, and 5]. Titanium dioxide nanoparticles have two very specific and interesting properties that give special applications to this material. These two properties are: the photocatalytic property and the hydrophilic property which rise to the properties of titanium dioxide nanoparticles in their self-healing surfaces, anti-microbial surfaces, water purifiers, and air purifiers. There are several novel methods used for the synthesis of titanium dioxide nanoparticles. The most important of these methods include hydrothermal, mechanical, mechanical Radiofrequency thermal plasma are chemical vapor condensation and sol-gel. Among the methods mentioned, the sol-gel method has the advantages of fine particle size distribution, chemical composition control and the creation of a thin layer on the surfaces. In 2007, Venkatachalam et al. Produced TiO_2 nanoparticles by sol-gel method. In this work titanium isopropoxide, acetic acid and water with specific molar ratio were used [6, 7].The results showed that this method is defective for the production of this powder due to its tendency to rapidly agglomerate against crystallization. However, it was found that high calcined temperature caused the formation of TiO_2 crystalline particles. Researchers are also worked on TiO_2 microstructural changes using ultrasound on the sol-gel technique. [2.8]. the results showed that the crystalline powder is fully formed in this process and the ultrasound waves accelerate the crystallization process. This saves time and energy. Fallah et al. (2014) studied the effect of curing temperature on the electrical and optical properties of TiO_2 nanoparticles in the presence of Niobium based sol-gel method. The results showed that the two-phase atmosphere in the atmosphere greatly increased the film's media attention. Also in this case the electrical resistance is also significantly reduced. Studies were also performed on the microstructural properties of TiO_2 obtained by sol-gel method in the presence of mercury ion and the effect of annealing temperature. The presence of mercury ions will lead to better nanostructure and growth. In addition, in the presence of mercury ions, the reflectance power of the film increases sharply. In 2015 Agartan et al. studied the initial water content and calcination temperature based on sol-gel method on the photocatalytic properties of solid TiO_2 nanoparticles. It has been found that increasing the initial water makes the powders more crystalline and easier to crystallize without sedimentation. The results showed that despite the low temperature of synthesis, the TiO_2 nanopowder was formed with anatase phase in spite of the low temperature of synthesis [9]. Also, with the increase in acetic acid, the faster anatase phase is formed and the formation energy is reduced. In view of the above, it is difficult to obtain TiO_2 nanoparticles that contain both anatase and rutile phases, as well as particles lacking agglomeration and have a good dispersion. Therefore, the aim of this study was to synthesize TiO_2 nanoparticles at rutile phases by sol-gel method and study The Optical and crystalline properties. Various nanoparticles can be obtained with appropriate dispersion phases and with fine aggregation [10, 11].

This work Prepare TiO_2 synthesized nanoparticles by acid catalyzed sol–gel technique, This work reports optical properties and band positions of TiO_2 nanoparticles under Ultraviolet-visible (UV-Vis) –light ,then found band positions by Fourier Transform Infrared Spectrophotometer (FTIR) spectroscopy .

. Material & Method

Synthesis of titanium dioxide nanoparticles TiO_2: 50 ml of $TiCl_4$ solution were slowly added to 200 ml of distilled water in an ice bath. After the addition completed, the mixture was stirred for 30 minutes at room temperature. The solution was heated in water bath for 90 minutes under refluxing. Then, it was filtered using vacuum pump and claimed at 600^oC in the muffle furnace for 2 hours [12].The used UV spectrometer min 1240 to carry out the optical properties like(absorbance ,absorption coefficient ,refractive index ,optical conductivity and electrical conductivity).And used Fourier Transform Infrared Spectrophotometer (FTIR) spectroscopy to locate the band positions .

Results

After preparing TiO_2 sample study the (optical and Band Positions) properties by used UV spectrometer beside and FTIR spectroscopy, the results are showing blow

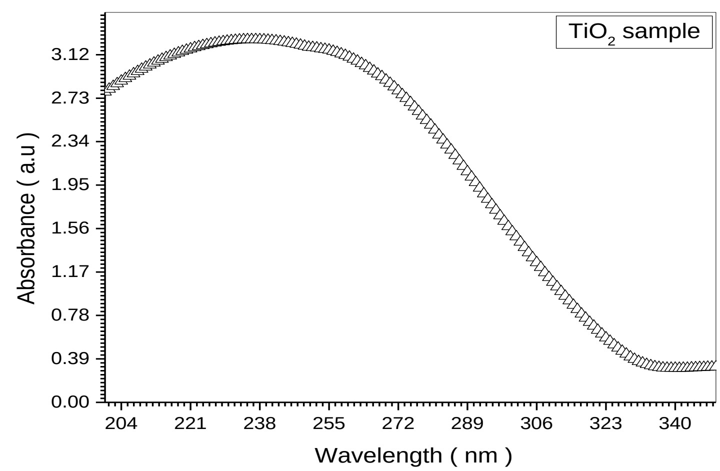
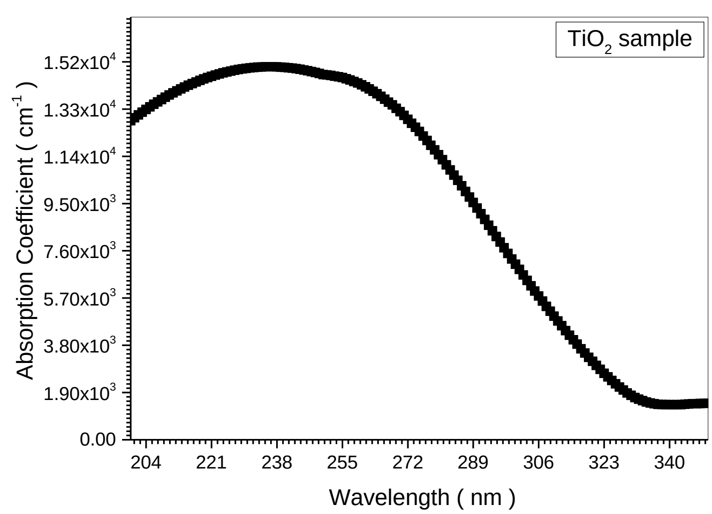
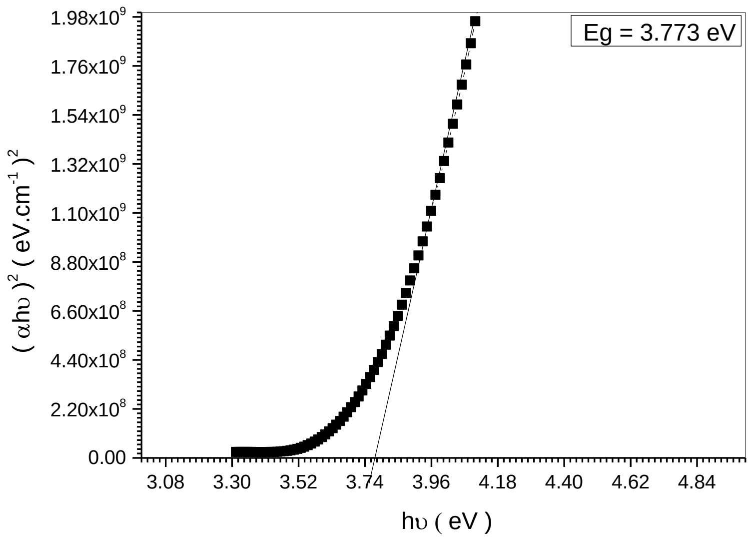


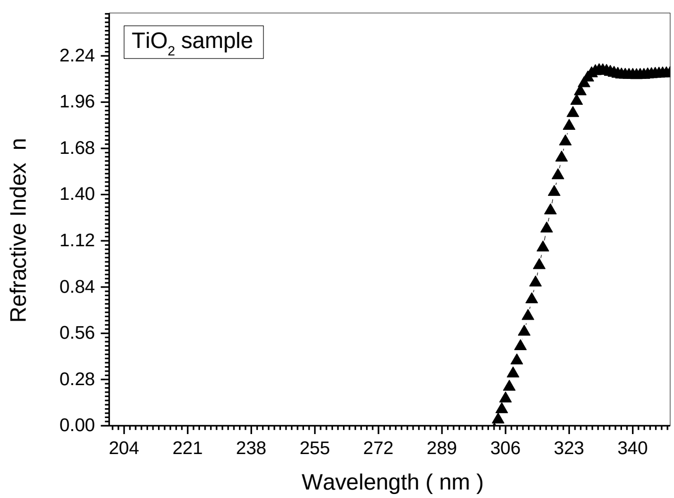
Fig (1) relation between absorbance and wavelengths of TiO_2 sample



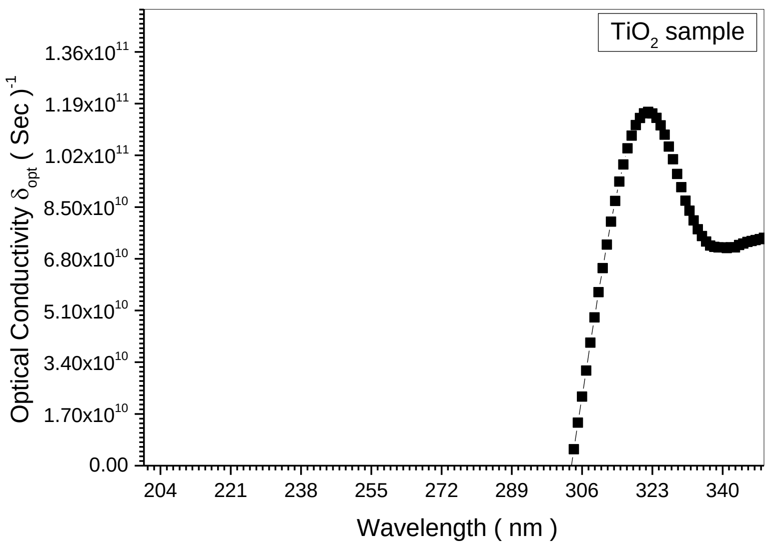
Fig(2) relation between Absorption Coefficient e and wavelengths of TiO_2 sample



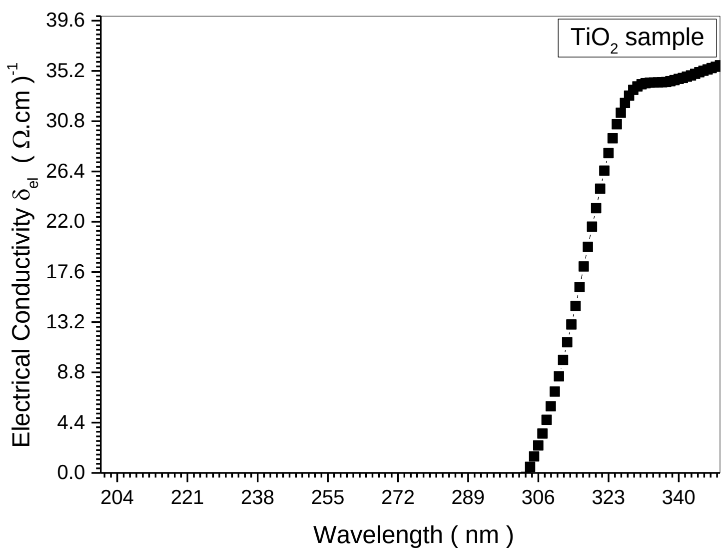
Fig(3) Optical Energy Band Gap of TiO_2 sample



Fig(4) relation between Refractive Index and wavelengths of TiO_2 sample



Fig(5) relation between Optical Conductivity and wavelengths of TiO_2 sample



Fig(6) relation between Electrical Conductivity and wavelengths of TiO_2 sample

The absorbance of TiO_2 sample studied using UV-VS min 1240 spectrophotometer . Show the resolute of absorbance show in fig (1). In fig. (1) shows the relation between absorbance and wavelengths of TiO_2 sample , it is in the reenged (200 - 350) nm the maxiumal value of absorbance in 240 nm crosponding photon energy 5.17 eV. The absorption coefficient (α) of the prepared sample of TiO_2 were found from the following relation $\alpha = \frac{2.303 x A}{t}$ where (A) is the absorbance and (t) is the optical legth on the sample . In fig (2) shows the plot of (α) with wavelength (λ) of TiO_2 sample , which obtained that the value equal $1.52x10^4$ cm^{-1} in the U.V region (240 nm) , this means that the transition must corresponding to a direct electronic transition, and the properties of this state are important since they are responsible for electrical conduction. The optical energy gap (Eg) has been calculated by the relation $(\alpha h\upsilon)^2 = C(h\upsilon - Eg)$ where (C) is constant. By plotting $(\alpha h\upsilon)^2$ vs photon energy (hυ) as shown in fig.(3) for prepared sample by TiO_2. And by extrapolating the straight thin portion of the curve to intercept the energy axis , the value of the energy gap has been calculated .In fig (5.3) the value of (Eg) of TiO_2 sample obtained was (3.773) eV. The refractive index (n) is the relative between speed of light in vacuum to its speed in material which does not absorb this light. The value of n was calculated from the equation $n = [\left(\frac{(1+R)}{(1-R)}\right)^2 - (1 + k^2)]^{\frac{1}{2}} + \frac{(1+R)}{(1-R)}$ Where (R) is the reflectivity. The variation of (n) vs (λ) for TiO_2 sample was shown in fig.(4). Fig (4) Show that relationsheep of TiO_2 prepared sample refractive index (n) spectra,which shows that the maximum value of (n) is (2.19) for TiO_2 samples at 330 nm . Also we can show that the value of (n) begin to decrease befor 330 nm and equal zero at 300 nm of region of spectrum . The optical conductivity is a measure of frequency response of material when irradiated with light which is determined using the following relation, $\boldsymbol{\delta_{opt}} = \frac{\alpha n c}{4\pi}$ Where(c) is the light velocity. The electrical conductivity can be estimated using the following relation $\boldsymbol{\delta_{ele}} = \frac{2\lambda\delta_{opt}}{\alpha}$ The high magnitude of optical conductivity ($1.17x10^{11}$ sec^{-1}) confirms the presence of very high photo-response of the TiO_2 sample prepared . The increased of optical conductivity at high photonenergies is due to the high absorbance of TiO_2 sample formand may be due to electron excitation by photon energy as it is shown in Figs (5) and (6) .

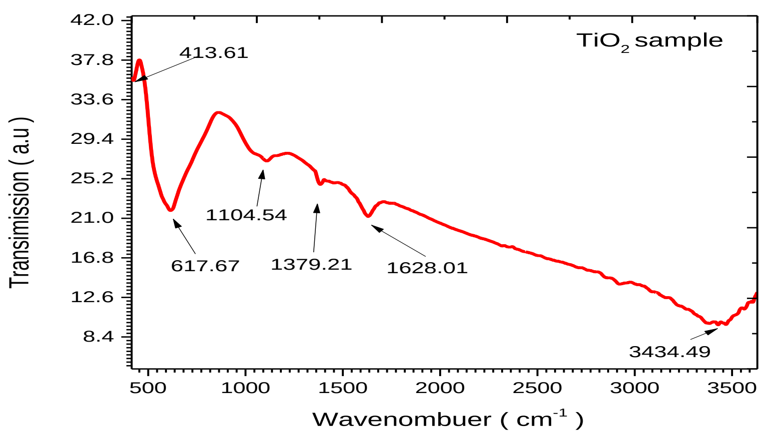


Fig (7) FTIR spectrum of TiO_2 sample

Table (1) Parameters of T iO_2 sample

No	Wavenumber (cm^{-1})	Functional Group	Wavenumber (cm^{-1})	Functional Group
1	415	metal-oxygen	600–500	C-I stretch
2	620	metal-oxygen	700–600	C - Br stretch
3	1105	Methyl Formate	(1300-1000)	C-C stretch
4	1380	Methane	1400-1300	C =O Bend
5	1630	Methyl Formate	1755-1650	C=O Stretch
6	3440	Methanamide	3500-2400	Hydrogen- bonded O-H Stretch

The infrared spectra of synthesized TiO_2 nano ferrite powders were recorded by mattson Fourier Transform Infrared Spectrophotometer in the range of 400 to 4000 cm^{-1} which shown in Fig(7) . The spectra of TiO_2 have been used to locate the band positions which are given in the Table (1) . In the present study the absorption bands ν1, ν2, ν3, ν4 , ν5, and ν6 are found to be around 4153cm^{-1}, 620 cm^{-1}, 1105 cm^{-1}, 1380 cm^{-1}, 1630 $cm^{-1}$and 3440 cm^{-1} respectively for all the compositions. The transmiattance bands within these specific limits reveal the formation of single-phase spinel structure having two sub-lattices tetrahedral (A) site and octahedral (B) site. The (ν1) band and band (ν2) around 415 and 620 cm^{-1} is caused by the metal-oxygen vibration in the tetrahedral sides. This difference in the spectral positions is due to the different values of metal ion-O^{-2} distances for octahedral and tetrahedral sites. The band (ν3) around 1105 is due to C-C stretch. The band (ν4) around 1380

cm^{-1} is associated with the O-H bending vibration .The band (v5) around 1630cm^{-1} is due to C= O stretching. (v6) around 3440 cm^{-1} is due to the stretching mode of H-O-H bending vibration of free or absorbed water which implies that the hydroxyl groups are retained in ferrites .

Conclusion

Synthesis of titanium dioxide nanoparticles by sol gel method ,the absorbance at reenged (200 - 350) nm ,maximal absorption coefficient value equal $1.52x10^4$ cm^{-1} at the U.V region (240 nm) ., and the energy band gap value of (Eg) equal (3.773) eV .the maximum value of refractive index (n) is (2.19) and optical conductivity ($1.17x10^{11}$ sec^{-1}) .

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