Study of Structure and Optical for Chemically Synthesized Titanium Dioxide Nanoparticles

P.B. RATHOD[1], K.R. NEMADE[2], S.A.WAGHULE[1]

[1]Department of Physics, Sant Gadge Baba Amravati University, Amravati 444 602, India.
[2]Department of Applied Physics, J D College of Engineering and Management, Nagpur 441 501, India.
Correspondence Author: sandeepwaghuley@sgbau.ac.in

Abstract

Titanium dioxide (TiO_2) nanoparticles were synthesized by a co-precipitation method. The synthesis was carried out at room temperature using titanium tetrachloride ($TiCl_4$) and NaOH as precursors. The structure of the TiO_2 nanoparticles were tested with X-Ray diffraction technique and it was formed to be crystalline with many strong peaks. The X-ray diffraction pattern confirmed the formation of TiO_2 nanoparticles phase with an excellent crystalline structure. The optical property concerning the absorption was studied for the chemically synthesized TiO_2 nanoparticles by using ultraviolet-visible spectroscopy. Scherrer equation is used for the determination of particle size, which was found to be 24 nm. Different optical parameters are estimated and discussed.

Keywords: *TiO_2 nanoparticles, Co-precipitation method.*

Introduction

Presently, titanium dioxide (TiO_2) nanoparticles, is one of the most widely studied material in the fields of photocatalysis [1-2], heterogeneous catalysis [3] and dye sensitised solar cells [4-5]. The TiO_2 crystal exists in mainly two forms: anatase and rutile. Anatase is thermodynamically metasTable and at high temperatures, anatase can be transformed irreversibly to rutile phase. Most of the researchers have paid greater attention to anatase TiO_2 than rutile TiO_2, because anatase phase of TiO_2 had been considered to be more active than rutile. Fujishima et al. used TiO_2 for photokilling tumour cells [6]. Regan et al. reported an efficient solar cell with TiO_2 particles coated with organic chromophore groups active under visible light [7]. Sonawane et al. studied the Fe-doped TiO_2 films for photodegrade of methyl orange in a solution after exposure to sunlight for several hours [8]. Wang et al. reported the anti-fogging and self-cleaning properties with developed highly hydrophilic TiO_2 surfaces [9]. Many researchers synthesized TiO_2 by various methods such as Watson et al used the sol-gel technique to coat magnetic particles with TiO_2 [10]. Yana et al. synthesized pure rutile nanotubes in NaOH water-ethanol solution starting from rutile-anatase TiO_2 particles by a hydrothermal process and shows that rutile phase TiO_2 nanotubes exhibited different optoelectronic properties than the TiO_2 [11]. Mozia et al. prepared modified titanate nanotubes via a hydrothermal method and focused on their application [12]. Dawson et al. subjected mixed phase TiO_2 powders with different compositions and particle sizes with NaOH by hydrothermal reaction [13]. The synthesis methods discussed above has some advantages as well as disadvantages. Co-precipitation is an easy and convenient approach to synthesize TiO_2 nanoparticles from aqueous solutions. It is observed that size, shape, and composition of the resulting particles highly depend on the reaction conditions.

In the present work, TiO_2 nanoparticles were synthesized by co-precipitation method. As synthesized TiO_2 nanoparticles were characterized by X-ray diffraction (XRD) technique. The indirect band gap of TiO_2 was determined through UV–VIS spectra.

Experimental Details

TiO_2 nanoparticles were synthesized by co-precipitation method using AR grade chemicals without further purification. The titanium tetrachloride ($TiCl_4$) and sodium hydroxide (NaOH) were used as starting materials. For synthesis, both chemicals were mixed in 1:1 M ratio at room temperature. The white precipitate so obtained was centrifuged and filtered with cellulose nitrate filter papers and washed several times by distilled water. The obtained product was dried at room temperature for 24 h and sintered at 100 °C for 24 h. The crystalline phase of sample was identified by using X-ray diffraction (XRD)technique. X-ray diffraction pattern was recorded using a Rigaku miniflex-II diffractometer with CuKα radiation (λ=1.541 Å) in the range 10°-70°. UV-VIS spectrum was recorded on Perkin Elmer UV spectrophotometer in the range 200–600 nm.

Result and Discussion

The XRD pattern of TiO_2 nanoparticles is depicted in Fig.1. The peaks appear in XRD pattern shows the structural purity of as-synthesized TiO_2 nanoparticles. The peaks position and marginal intensity difference exactly indexed to JCPDS card-01-070-7348, which reflects that TiO_2 in anatase phase. No other impurity peak appears in the pattern. The average crystallite size of TiO_2 nanoparticles was calculated using the Scherer's equation (1) [14].

$$D=K\lambda/(\beta COS\theta) \qquad (1)$$

where, D is the crystallite size, K is the shape factor, which can be assigned a value of 0.9 if the shape is unknown, θ is the diffraction angle at maximum peak intensity, and β is the full width at half maximum of diffraction angle in radian. When applied to some prominent peaks, Eq. (1) leads to the average crystallite size of about 24 nm.

The optical characteristics of as-synthesized TiO_2 nanoparticles were investigated in wavelength range 200-600 nm, which further used for study of absorption coefficient and indirect band gap. The absorbance spectra for TiO_2 nanoparticles are shown in Fig.2. This spectrum reveals that the maximum absorption peak appears in UV region. Many applications of the materials depend upon its indirect band gap values. The relation between absorption coefficient (α) and incident photon energy (hν) can be expressed as Eq. (2).

It is the indirect band gap of TiO_2 nanoparticles and found to be 3.1 eV by substituting the exponent value n = 2 in Eq. (2) [15]

$$\alpha = A(h\nu - Eg)n/h\nu \qquad (2)$$

where, α is absorbance, A is a constant and Eg is the band gap of the material. The exponent n depends on the type of the transition; its value is 1 for direct band gap and 2 for indirect band gap.

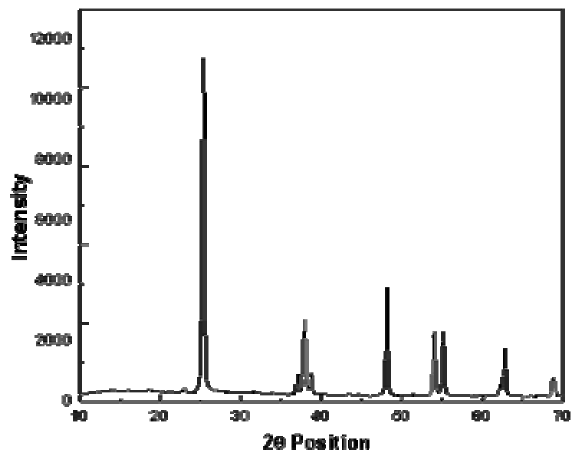

Fig. 1: XRD pattern of TiO_2 nanoparticles.

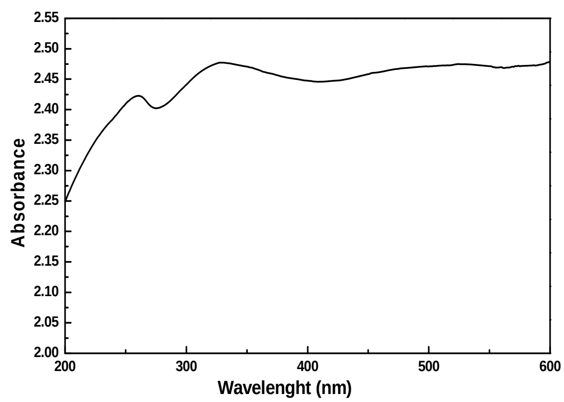

Fig. 2: The optical absorbance of TiO_2 nanoparticles.

Fig. 3 shows the variation of extinction coefficient as a function of a wavelength. The extinction coefficient (K) is a measure of the fraction of light lost due to scattering and absorption per unit distance of the penetration medium. The extinction coefficient is computed in the sample during the exposure of UV spectra by using the relation between absorption and wavelength. Extinction coefficient (K) is determined by using Eq.(3) [16].

$$K = \alpha\lambda/4\pi \qquad (3)$$

where, α is absorption and λ is wavelength (nm). The curve of extinction coefficient as a function of wavelength shows that scattering increases gradually from 200 nm to 325 nm for constant distance of the penetration medium

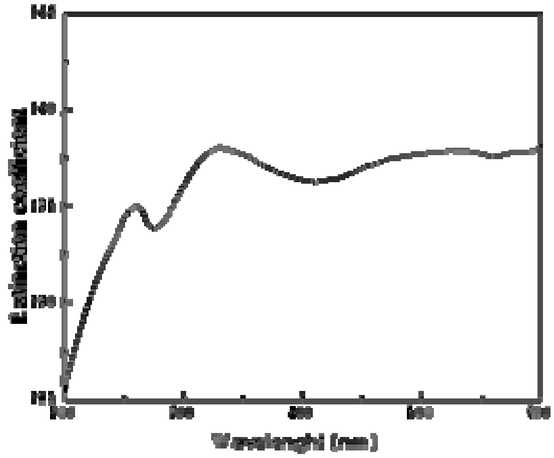

Fig. 3: Variation of extinction coefficient vs. wavelength.

Fig. 4 shows the variation of $(\alpha h\upsilon)^2$ as a function of E(ev) for TiO_2 nanoparticles. It can be observed from figure that energy gap equal to 3.1 eV for the value of exponent n=2.

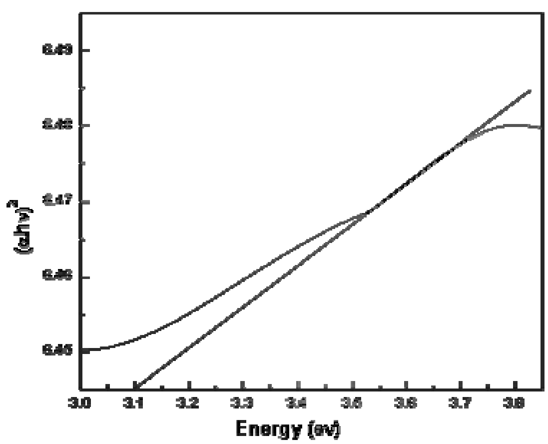

Fig. 4: Variation of $(\alpha h\upsilon)^2$ versus energy (eV) for TiO_2 nanoparticles.

Conclusions

In summary of present work, we have successfully synthesized TiO_2 nanoparticles by co-precipitation method. An average particle size of the resulting TiO_2 nanoparticles was found to be 24 nm computed from XRD analysis by using scherer's equation. An indirect band gap of TiO_2 nanoparticles was found to be 3.1 eV. The optical constants absorbance coefficient and extinction coefficient of these sample was determined using absorbance spectra. The estimated optical band gap energy is an accepted value for the photocatalytic activities in visible light and also for application in the photovoltaic and optical devices. The co-precipitation used in this paper is a simple, useful, and an economic method to synthesized TiO_2 nanoparticles.

Acknowledgements

Authors are very much thankful to the Head, Department of Physics Sant Gadge Baba Amravati University Amravati for providing necessary facilities.

References

[1] H. Lin, C. P. Huang, W. Li, C. Ni, S. I. Shah, Y. H. Tseng, Applied Catalysis B-Environmental,68(1), 2006, 1-11.

[2] A. Fujishima, K. Honda, Nature, 238(7), 1972, 37 – 38.

[3] M. Valden, X. Lai, D. W. Goodman, Science, 281(11), 1998, 1647-1650.

[4] K. Hirano, E. Suzuki, A. Ishikawa, journal of Photochemistry and Photobiology A: Chemistry 136 (3), 2000, 157-161.

[5] A. Kay, M. Gratzel, Solar Energy Materials and Solar Cells 44(1), 1996, 99–117.

[6] A. Fujishima, J. Ohtsuki, T. Yamashita, S. Hayakawa Photomed Photobiol, 8(45), 1986, 45–46.

[7] O. Regan, M. Gratzel, Nature, 1991(353), 1991, 737–740.

[8] R. S. Sonawane, B. B. Kale, M. K. Dongare, Mater Chem. Phys, 2004(85), 2004, 52–57.

[9] R. Wang, K. Hashimoto, A. Fujishima, Nature, 1997(388), 1997, 431–432.

[10] S. Watson, D. Beydoun, R. Amal, Journal Photochem Photobiol A Chemistry, 2000(148), 2000, 303–311.

[11] J. Yana, S. Fenga, H. Lua, Mat Sci Eng B, 2010(172), 2010, 114–120.

[12] S. Mozia, Catalysis Today, 2010 (156), 2010, 198–207.

[13] G. Dawson, W. Chen, T. Zhang, Solid State Sci, 2010(12), 2010, 2170–2176.

[14] S. A. Waghuley, S. M. Yenorkar, S. S. Yawale, S. P. Yawale, Sens. Actuators, 2008(128), 2008, 366-373.

[15] K.R. Nemade, S.A. Waghuley, Results in Physics, 3(3), 2013, 52–54.

[16] K.R. Nemade, S.A.Waghuley, International Journal of Metals, 2014 (1) 2014, 1-4.