Facile Synthesis and Characterization of TiO_2 Nanoparticles for Photovoltaic Applications

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***Abstract*— TiO_2 nanoparticles were synthesized by hydrothermal method. The as prepared nanoparticles were calcined at 400º C. The samples were characterized by XRD, SEM. Surface morphological studies obtained from SEM micrograph showed the particles with the spherical shapes are anatase in nature. The Crystalline size of TiO_2 powder (TNP1 and TNP2) has obtained is ~39nm, 28 nm for anatase at 400 ºC by controlling the acidity.**

***Keywords*— TiO2 particles; ;;**

I. INTRODUCTION

TiO_2-based nanostructured materials have been extensively studied over the past three decades due to its low toxicity/cost, chemical stability, excellent photocatalytic activity, and long lifetime of electron/hole pairs. However, one of the main disadvantages of TiO_2 is its large band gap (about 3.2 eV) can absorb only the ultraviolet (UV) light contained in a solar spectrum and the inability to utilize visible light limits the efficiency of photocatalytic degradation of organic pollutants .TiO_2 has three crystalline polymorphs: anatase, rutile and brookite. Anatase and brookite are in meta stable phase but can be transformed into rutile on heating. For photocatalytic and solar cell applications, anatase phase is more preferable.TiO_2 nanostructures have been synthesized by coprecipitation, sol-gel , solvothermal and hydrothermal synthesis methods.(2-6) Among these methods, the alkaline hydrothermal method is relatively simple method and produce high yields of TiO_2 nanoparticles. The higher photo conversion efficiency could be achieved by smaller TiO_2 particles. However, the size, the morphology, and the structural properties of TiO_2 nanostructures depend on the TiO_2 precursors and reaction parameters, such as the reaction temperature, the reaction time, and the solution pH during the reaction. In this paper we prepared TiO_2 nanoparticles by hydrothermal method with different pH values. It is found that the TiO_2 crystallinity and morphology is improved when pH is varied.

II. EXPERIMENTAL DETAILS

TiO2 nano-powders were prepared via Hydrothermal method using titanium tetraisopropoxide, distilled water, ethyl alcohol and Citric acid as the starting materials. The drop wise addition of titanium isopropoxide (TTIP) was made to the solution of distilled water, ethyl alcohol and Citric acid under constant magnetic stirring. The mixture was further stirred for about 2 h and then transferred to the stainless steel auto clave with teflon lining. The sealed auto clave was subjected to thermal treatment at a steady temperature of 150 °C for 3 hour. The auto clave was removed from the oven and then naturally allowed to come to room temperature. The final product was filtered and dried in open atmosphere. Further it was calcined at 400º C for 2hour. The samples were prepared with two different pH values. The samples were named by TNP1 and TNP2.

III. RESULTS AND DISCUSSION

A. Structural analysis

The XRD measurement was performed under radiation of Cu Kα 1.54060 Å. Based on the diffractograms shown in figure 1 and 2, it can be seen that both TiO_2 crystallites are in the anatase phase whereas the highest peaks of both TiO_2 were found at (101) crystal plane.

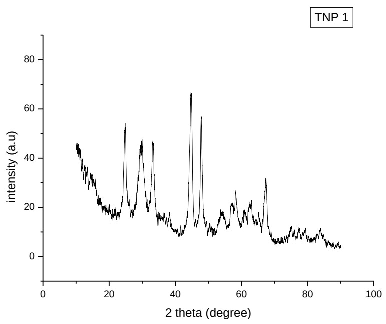

Fig. 1. XRD pattern of TNP 1 TiO_2 particles

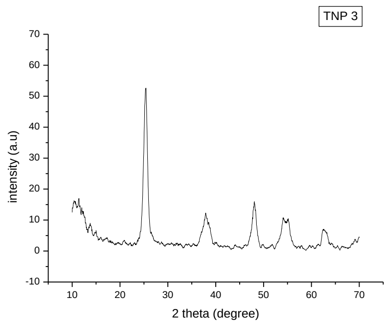

Fig. 2. XRD pattern of TNP 3 TiO_2 particles

Scherrer formula in the following equation was used to calculate the lower bound of the particle grain size.

$$\tau = \frac{k\lambda}{\beta \cos\theta} \quad \text{------------------ (1)}$$

Where τ is the mean size of the crystals, *k* is the shape factor (with typical value around 0.9), λ is the x-ray wavelength, β is the line broadening at half the maximum intensity (FWHM), and θ is the Bragg angle. The crystallite size of TNP 1 and TNP 3 are calculated according to the Scherrer equation, was found to be 39 nm and 28 nm, respectively. The broadening of the peaks clearly shows the small size of the nanoparticles. Increasing the pH value the particle size was reduced; it was improve the efficiency of the device.

B. *Surface morphological analysis*

As the surface to volume ratio is the dominant factor in nanostructured materials, probing the materials surface features is the prerequisite for many important applications. The surface morphology of the as prepared samples was examined by SEM. Figure 3, 4 shows the SEM images of the TiO_2 nanoparticles with grain sizes 40-60 nm approximately. They reveal the formation of nanocrystalline materials and show the aggregates of nanoparticles with variable sizes. TiO_2 nanoparticles are prone to aggregate due to the large surface area and high surface energy.

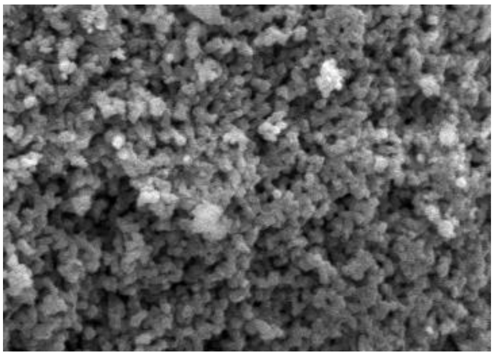

Fig. 3. SEM image of TNP1 sample

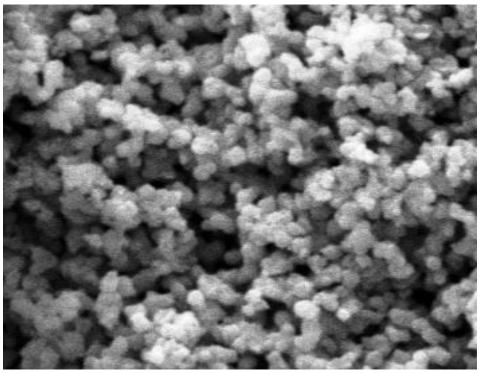

Fig. 4. SEM image of TNP 3 sample

SEM images exhibits the inprovement of praticle grouth depends upon the pH value. Fig.4. Shows the uniform sherical paticles, Increasing the pH value, the morphology of the particles were changed.

C. *UV Visible Spectroscopic analysis*

UV-vis spectrophotometer measurements were performed to compare the optical characterizations between two types of TiO_2. Figure.5 and 6, shows the optical absorption of TiO_2 nanoparticles (TNP 1 and TNP 3). It can be seen that TNP 3 generally has better absorption ability upon a broader wavelength interval. The blue shift in the exciton absorption clearly indicates the quantum confinement property of nanoparticles. In the quantum confinement range, the band gap of the particles increases resulting in the shift of the absorption edge to lower wavelength, as the particle size decrease.

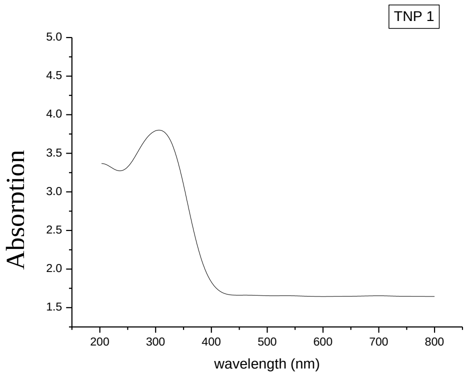

Fig 6. Shows the absorption nspectra of TNP 1 TiO_2 particles

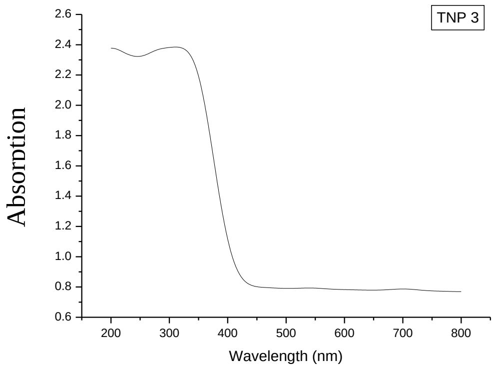

Fig 6. Shows the absorption nspectra of TNP 3 TiO_2 particles

$$\alpha h\gamma = A(h\gamma - E_g)^n \qquad \text{------------------ (2)}$$

Where A is constant and Eg is a band gap. The value of n is ½ or 2 depending on presence of the direct allowed and indirect allowed transitions. The prepared particles band gaps are 3.1 eV and 3.00 eV, respectively.

D. I-V Study

Room temperature resistivity of the TiO_2 nanoparticles were determined by the standard and most widely using method the four probe technique.

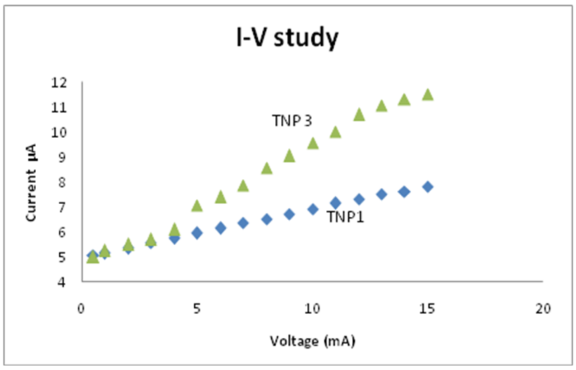

Fig 7. Shows the I-V of Difffernt pH nano particles

Current is gradually increased with the voltage. The I-V Characterization and resistivity are depending upon the pH value of the TiO_2 nano particles.

IV. CONCLUSION

TiO_2 nanoparticles were synthesized by hydrothermal method at pH 1 and 3. The as prepared nanoparticles were calcined at 400° C. The Crystalline size of TiO_2 powder (TNP1 and TNP 3) has obtained is ~39nm, 28 nm for anatase at
400 ºC showed that crystallinity and morphology is improved when pH is increased. The optical band gaps of the prepared TiO_2 particles were 3 and 3.1 eV. I V characterization results also reveals that the efficiency was improved when pH is increased.

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