



## STRUCTURAL, OPTICAL AND PHOTOCATALYTIC PROPERTIES OF SOL-GEL SYNTHESIZED MESOPOROUS TiO<sub>2</sub> THIN FILM

Simin Janitabar Darzi, Akram Hosseinian, Ali Reza Mahjoub\*

Department of Chemistry, Tarbiat Modares University, 14115-175, Tehran, Iran, [Mahjouba@modares.ac.ir](mailto:Mahjouba@modares.ac.ir)

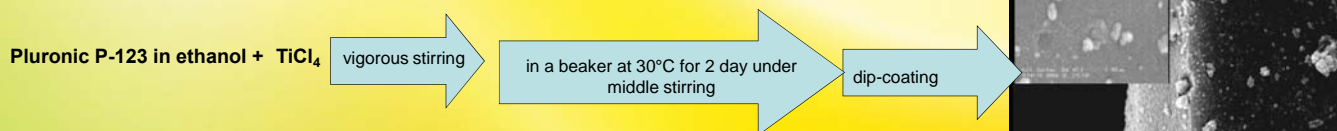
### Abstract

nanostructured TiO<sub>2</sub> thin film was fabricated using TiCl<sub>4</sub> and P-123 as raw material and surfactant, respectively. The film was produced by sol-gel dip coating procedure. Characterization of the product was carried out by means of XRD, SEM, BET specific surface areas, TG, and UV-vis absorption spectroscopy. Film is transparent and has a wormlike mesostructured with high surface area. It is about 2 μm thick and is composed of closely packed anatase particles. The estimated band gap value of TiO<sub>2</sub> thin film in the present work is 3.7 eV (according to quantum size effect). The film has excellent photocatalytic efficiencies and more than 70% of Crystalviolet dye was decolorized in 60 minutes.

**Key Words:** Optic, Quantum size effect, TiO<sub>2</sub>, Thin film, photocatalysis.

### Introduction

Nanosized and nanoporous photocatalyst particles have high specific surface area and exhibit significant activity in degradation of dyes and other effluents. Moreover, nanostructured materials exhibit quantization effect [1]. In this paper, we describe the synthesis of a nanoporous TiO<sub>2</sub> thin film by sol-gel templated process. The film was produced dip coating procedure due to its simple technique as well as relatively low cost. Then influence of high porosity of anatase film on the optical and physicochemical properties investigated and finally its photocatalytic activity was studied using artificial UV light for degradation of the Crystalviolet dye.



### UV-VIS spectroscopy and optical measurements

The band gap of the TiO<sub>2</sub> thin film reveals 0.3 eV shift from value reported in literature for anatase thin film. It could be due to quantum size effects. A mathematical treatment using a quantum mechanical approach gives the relationship between band gap shift compared to bulk anatase ( $\Delta E_g$ ) and the radius of quantum-sized particles. The particle diameter of Synthesized TiO<sub>2</sub> was calculated to be 1.37 nm.

The **refractive index** can be calculated from the above values with the help of the following relation :

$$n = \sqrt{N + \sqrt{N^2 - n_0^2 n_1^2}}$$

Where

$$N = \frac{n_0^2 + n_1^2}{2} + 2n_0 n_1 \frac{T_{\max} - T_{\min}}{T_{\max} T_{\min}}$$

where  $n_0$  and  $n_1$  are the refractive indices of air and substrate, respectively,  $T_{\max}$  is the maximum envelope and  $T_{\min}$  is the minimum envelope. The refractive index obtained in the present work is 1.54 which is in good agreement with the earlier reports on TiO<sub>2</sub>. The value of refractive index is lower than that of the bulk TiO<sub>2</sub> (anatase = 2.54), probably due to the nanosize of the grains

The **porosity percentage** of prepared TiO<sub>2</sub> thin film and bulk anatase TiO<sub>2</sub> was calculated to be 67% and 19.8%, respectively using the following equation :

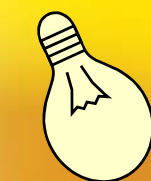
$$\% \text{ Porosity} = \left[ 1 - \left( \frac{n^2 - 1}{n_d^2 - 1} \right) \right] \times 100$$

where  $n_d$  is the refractive index of pore-free TiO<sub>2</sub> (2.52)

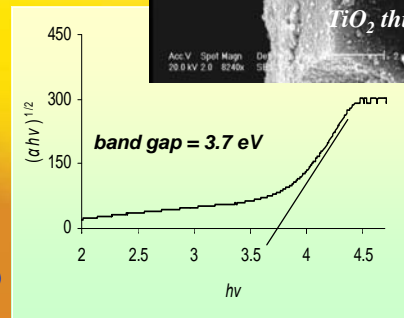
A mathematical treatment using a quantum mechanical approach gives the relationship between band gap shift compared to bulk anatase ( $\Delta E_g$ ) and the **radius (R) of quantum-sized particles**, expressed as:

$$\Delta E_g = \frac{h^2}{8\mu R^2} - \frac{1.8e^2}{\epsilon R}$$

where  $h$  is Planck's constant,  $\mu$  is the reduced mass of the electron and the hole ( $1/\mu = 1/m_e^* + 1/m_h^*$ ) in the semiconductor,  $e$  is the electron charge, and  $\epsilon$  is the dielectric constant of the semiconductor, Kormann et al. cited  $\epsilon = 1.84$  and calculated a value of  $\mu = 1.63m_e$  ( $m_e$  is the electron rest mass) [2]. The **particle diameter** of Synthesized TiO<sub>2</sub> was calculated to be **1.37 nm**.

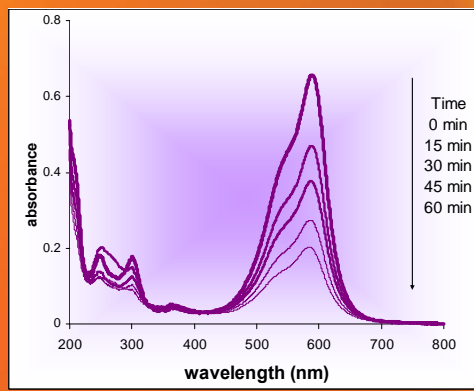


UV lamp (30 W)



XRD pattern of the prepared TiO<sub>2</sub> powder shows the diffraction peaks can be indexed to the tetragonal structured anatase. specific surface area = 124.6 m<sup>2</sup>g<sup>-1</sup> N<sub>2</sub>-adsorption isotherm as a function of P/P<sub>0</sub> was revealed that the prepared thin film is mesoporous (isotherm is of type IV).

Aerated aqueous solution of Crystalviolet dye (5 ppm)



Spectral changes that occurs during photocatalysis of aerated aqueous solution of Crystalviolet dye

### References

- [1] A. D. Yoffe, Adv. Phys., 42 (1993) 173.
- [2] C. Kormann, D.W. Bahnemann, M.R. Hoffmann, J. Phys. Chem. 92 (1988)5196.