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Optical Properties of TiO_2 Thin Film: Dip Coating Method

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Titanium dioxide (TiO_2) thin films have found countless applications, and the fabricated films have different structures that can lead to additional or enhanced properties. The aim of this paper is to show the preparation and optical characteristics of TiO_2 thin films obtained by sol-gel dip coating. TiO_2 is a well-known semiconductor with possible applications in optoelectronics, such as solar cells, light emitting diodes, liquid crystal displays, etc. The various optical parameters such as refractive index, extinction coefficient, band gap and optical conductivity were calculated using different formulas with respect to wavelength in the UV-visible region. It is found that the direct band gap transition comes out to be 3.34 eV, whereas the refractive index and extinction coefficient show variation in the UV-visible range. TiO_2 thin film shows Ti–O–Ti vibrational modes from IR spectra. This sort of research work will help us to find the best thin film coating technology for designing optoelectronic devices. This type of optical properties helps to optimize the best material/property relationship for promising devices.

Keywords: Optoelectronics, Dip coating, Thin film, TiO_2, Band gap.

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1. INTRODUCTION

In recent years, with the beginning of nanotechnology, powder and films of TiO_2 have been widely explored due to its new properties obtained by decreasing the particle size. This is called quantum confinement (QC), that is why, it shows high transmittance, high refractive index, and better optoelectronics properties. Titanium dioxide (TiO_2) is a well-known multifunctional semiconductor and usually commercialized in rutile or anatase phases with a tetragonal crystal structure. Thus, TiO_2 has a variety of applications, such as optical filters [2], gas sensors [3], ceramic membranes [4], waveguides [5], photo catalysts [6], and dye sensitized solar cells [7].

A number of techniques such as electron beam evaporation [8], DC magnetron sputtering [9], chemical vapor deposition [10] and sol-gel process [11] have been reported in the literature to obtain thin films of TiO_2. Films produced by these techniques are non-stoichiometric and non-uniform, and also expensive equipment is needed. Among these techniques, sol-gel dip coating process is an industrially promising technique for the preparation of thin films on large-area substrates as it offers advantages in terms of cost, low consumption of energy, low material consumption rate, simplicity and speedy deposition on small, as well as large, area substrates with good homogeneity without the requirement of expensive equipment [12].

In this paper, we report the deposition of TiO_2 films on glass substrate by sol-gel dip coating technique. We have studied the optical properties of TiO_2 film for optoelectronic applications.

2. EXPERIMENTAL SECTION

A 0.5 M TiO_2 sol was prepared by partial hydrolysis and polycondensation of titanium tetrabutoxide with water using isopropyl alcohol (IPA) as a solvent and HNO_3 as a catalyst. Titanium tetrabutoxide and water have been taken in 1:1 molar ratio [13]. Hydrolysis and polycondensation of titanium tetrabutoxide proceed according to the scheme depicted in Fig. 1a. Prior to sol-gel dip coating, the glass substrates were cleaned by a mild soapy solution and rinsed thoroughly with distilled water followed by boiled water. Finally, the solution was dropped onto glass substrates, as shown in Fig. 1b. The films thus prepared were inserted into a muffle furnace and kept at 450 °C for 10 min in order to evaporate the organic material. Fig 1c depicts the required stable film.

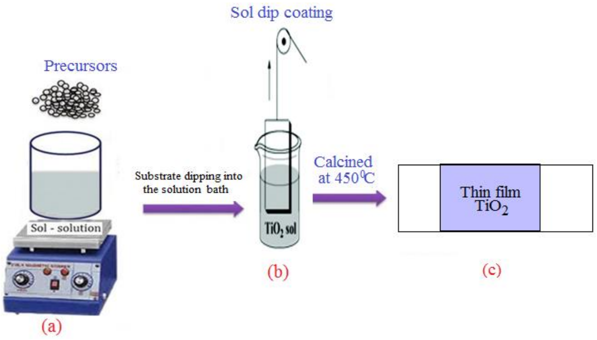

Fig. 1 – Sol-gel assisted dip coating process with muffle treatment at 450 °C

All characteristic measurements were carried out at room temperature in air. UV-visible and IR spectrosco-

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py characterization techniques were used to analyze the optical properties.

3. RESULTS AND DISCUSSION

3.1 Optical Properties

From the absorption edge, we can calculate the material band using the known Einstein photon energy relation [14]:

$$E_g = \frac{hc}{\lambda s}, \tag{1}$$

$$E_g = \frac{1240}{\lambda_s}\,\text{eV}, \tag{2}$$

where h is the Planck constant, c is the velocity of light, and λ_s (371 nm) is the excitonic absorption edge. The energy band gap is calculated to be ~ 3.31 eV. This value is suitable for optoelectronic devices like LEDs, solar cells, sensors, etc.

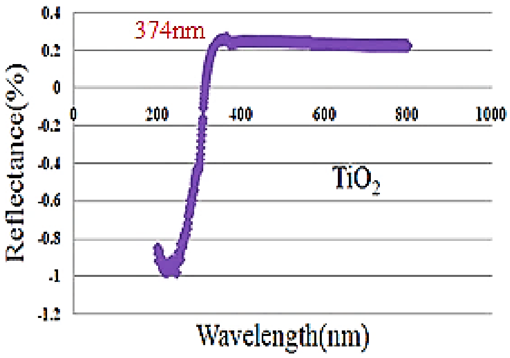

Fig. 2 – Reflectance spectra versus wavelength of TiO$_2$ thin film

3.2 Refractive Index and Extinction Coefficient

The information of the refractive index (n) and extinction coefficient (k) plays a significant role because these parameters basically give information about the suitability of the material for the fabrication of various optoelectronic devices and were obtained from reflectance data (not shown here). The refractive index (n) and extinction coefficient (k) were calculated by using below relations [15]

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}}, \tag{3}$$

$$k = \frac{\alpha\lambda}{4\pi}, \tag{4}$$

where λ is the wavelength of the incident photon, α is the absorption coefficient and R is the reflectance.

Fig. 4 shows the variations of the refractive index and extension coefficient versus the wavelength of TiO$_2$ film. The refractive index increases and the extinction coefficient decreases with increasing wavelength up to 400 nm, after which they remain constant. The magnitude of the refractive index is 1.2, and the extinction coefficient is 4.1×10^{-8}. Hence this type of variation for n and k in the UV-visible region makes them proficient for designing optoelectronic devices [16, 17].

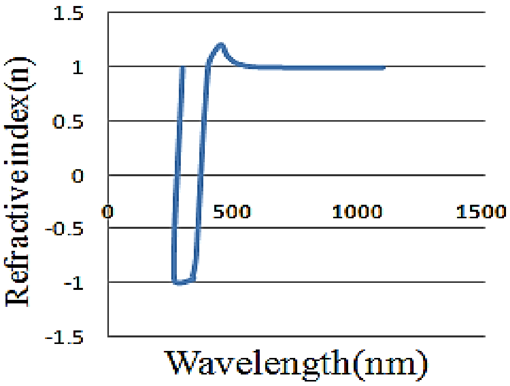

Fig. 3 – Variation of the refractive index spectra versus the wavelength of TiO$_2$ thin film

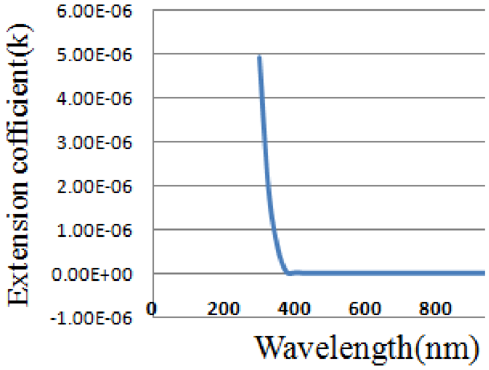

Fig. 4 – Variation of the extinction coefficient versus the wavelength of TiO$_2$ thin film

3.3 Optical Conductivity

The optical conductivity (σ_{opt}) is defined as a measure of optical response of a material [19] and is given by the relation:

$$\sigma_{opt} = \frac{\alpha n c}{4\pi}, \tag{5}$$

where c is the speed of light.

The optical conductivity is of the order of 10^{-4} s^{-1} and decreases significantly with increasing wavelength. The optical conductivity starts to decrease exponentially mainly due to a decrease in the electron extinction by photon energy which leads to a decrease in the electron transfer through materials at higher wavelength. The optical conductivity values at higher wavelengths remains constant due to low reflectance of the films.

3.4 FTIR Spectra Analysis

Fig. 5 presents the IR transmittance spectra of TiO$_2$ thin film recorded at room temperature in the 4000-400 cm^{-1} region. The weak, broad asymmetric stretching mode of surface-adsorbed moisture and hydroxyl bonding groups on their surface superimposed by vibration-rotational peaks in the 3800-3500 cm^{-1} region and a very weak component of the adsorbed CO$_2$ antisymmetric stretching peak at 2357 cm^{-1} are obtained in this film spectra [20, 21]. TiO$_2$ (anatase phase) [22, 23] thin film IR transmittance spectra, the characteristic metal-oxygen stretching modes of bridging of Ti–O–Ti, and Ti–O vibrations are observed in the 900-

400 cm^{-1} region and TiO_2 IR transmittance spectra, respectively. The peaks at 790 and 715 cm^{-1} arise from the stretching modes of bridging O–Ti–O and Ti–O–Ti bonding groups respectively in anatase phase of TiO_2.

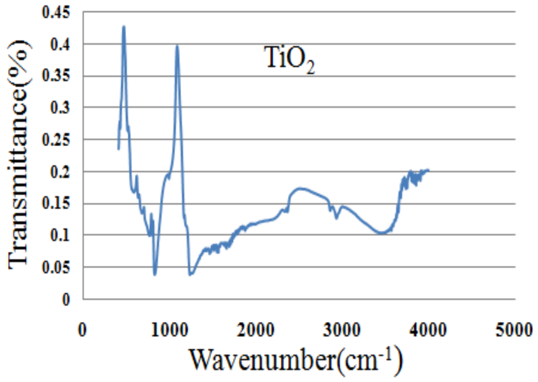

Fig. 5 – FTIR Spectra of TiO_2 thin film

4. CONCLUSIONS

The optical properties of TiO_2 thin films have been investigated including the refractive index, extinction coefficient, and band gap using absorbance data. The energy band gap is calculated from the Einstein relation and is found in the range of 3.34 eV. The refractive index and extinction coefficient have been found varied along with the optical conductivity up to a wavelength of 400 nm. So, the study reveals that dip coating is a simple technique for depositing TiO_2 thin film similar to wide band gap materials that are useful materials for solar cell applications.

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Оптичні властивості тонкої плівки TiO_2: нанесення покриттів методом занурення

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Тонкі плівки діоксиду титану (TiO_2) знайшли широке застосування. Виготовлені плівки мають різну структуру, що може призвести до додаткових або покращених властивостей. Мета даної роботи полягала у виготовленні та вивченні оптичних характеристик тонких плівок TiO_2, отриманих зануренням у золь-гель. TiO_2 є добре відомим напівпровідником з можливістю застосування в оптоелектроніці, наприклад, в сонячних елементах, світлодіодах, рідкокристалічних дисплеях, тощо. Різні оптичні параметри, такі як показник заломлення, коефіцієнт екстинкції, заборонена зона та оптична провідність, були розраховані за різними формулами залежно від довжини хвилі в УФ та видимій областях. Встановлено, що прямий перехід забороненої зони складає 3,34 еВ, тоді як показник заломлення та коефіцієнт екстинкції змінюються в УФ-видимому діапазоні. Тонка плівка TiO_2 демонструє коливальні моди Ti–O–Ti з ІЧ-спектрів. Дана дослідницька робота допоможе нам знайти найкращу технологію покриття тонких плівок для конструювання оптоелектронних пристроїв. Такі оптичні властивості допомагають оптимізувати найкраще співвідношення матеріал/властивість для перспективних пристроїв.

Ключові слова: Оптоелектроніка, Покриття зануренням, Тонка плівка, TiO_2, Заборонена зона.