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REGULAR ARTICLE

Calculations of Refractive Index Using Optical Band Gap: TiO_2 Spray Pyrolysis Thin Films

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Spray pyrolysis technique has been applied to deposit a broad range of thin films, which are used in various devices such as solar cells, sensors, and solid oxide fuel cells. Spray pyrolysis is one of the most common, inexpensive, simple, and quite versatile methods used for synthesizing submicron and spherical-shaped luminescent materials multicomponent oxide thin films. In this paper, spray pyrolysis TiO_2 thin films has been deposited on glass substrates and kept at different temperature to reveal its optical properties by the help of UV-visible spectroscopy. Refractive index (n) of TiO_2 thin films as wide semiconductor has been calculated using optical energy gap (E_g). The calculated values of refractive index from the new relations have been compared with the values reported by different researchers; an excellent agreement has been obtained between them. The material identification was confirmed from X-ray diffraction techniques and first derivative of transmission spectra's has been plotted that gives band gap value of films respectively.

Keywords: TiO_2, Spray pyrolysis, Band gap, Refractive index.

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1. INTRODUCTION

Refractive index and band gap of metal oxide semiconductors have been important parameter to study for semiconductors. This is because of their potential applications in a variety of Opto-electronic devices such as non-linear optics, light emitting diodes, photo-voltaic cells, photo-detectors, lasers, modulators, Integrated circuits and filters. Different researchers [1] have discussed various structural properties such as optical electronic and elastic of these semiconductors.[2]. In this direction Titanium dioxide(TiO_2), being an excellent n type semiconductor is getting a lot of attention for its wider band gap energy of more than 3 eV and distinct functionalities[3, 7]. Several techniques have been employed to synthesize the metal oxide composites such as sputtering, dip coating, electron beam evaporation, chemical vapour deposition, sol-gel process[8, 11] etc. These techniques are often costly and time consuming. In contrast, spray pyrolysis technique has been a cost effective and an efficient method while producing thick films over large areas with superior reproducibility and uniformity [12]. Readdy, Here have also attempted to obtained relation between n and E_g. In this paper we developed linear relationship between refractive index, optical energy gap. A correlation between band gap and refractive index is a subject of intensive research in recent times. Refractive index of a material is known to decrease with energy gap. There have been many attempts to find a suitable relationship both empirical and semi empirical between these two physical quantities. This paper reports the calculation of band gap helps to find out refractive index.

2. EXPERIMENTAL SECTION

The TiO_2 solutions were prepared with 0.24 M concentration of (TTIP) and the acetylacetone stabilizer waadded drop by drop to obtain yellow solution [8, 11]. The glass substrates were cleaned with diluting nitric acid, distilled water and finally with acetone. The TiO_2 solutions were deposited by spray pyrolysis technique onto glass substrates at 450 °C during 15 min with spray rate of 1 mL/ min to obtain anatase and rutile phases of TiO_2 thin films.TiO_2 thin films were deposited onto ordinary glass substrates at different substrate temperature using ultrasonic spray pyrolysis method.

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3. RESULTS AND DISCUSSIONS

3.1 XRD Analysis

The X-ray Diffraction (XRD) measurements were performed on TiO_2 thin film using a diffractometer (Bruker Axs D8 Advance, Germany). CuK_α radiation ($\lambda = 1.54$ Å) was used at a voltage of 40 kV and a current of 25 mA to reveal the exact composition and phase identification. Fig. 1 shows the XRD pattern of spray pyrolysis thin film and the diffraction pattern consists of peaks (101)A, (110)R, (101)R, (004)A, (200)R, (111)R, (210)R, (200)A, (101)R and (211)R for anatase phase and rutile phase of TiO_2 respectively. All the peak positions have been verified as mentioned in JCPDS Card Nos.86115TiO_2 [14] respectively. The lattice parameters are $a = 3.785$ and $c = 9.513$ and grain size (D) is 33.31 nm for most intense peak and has been calculated using formulas mentioned in the reference [15, 16].

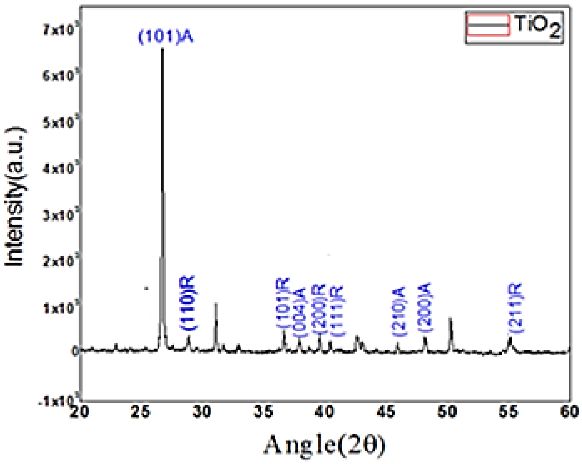

Fig. 1 – XRD pattern of TiO_2 thin film

3.2 Optical Transmittance Study

Figure 2 represents the optical transmittance versus wavelength, and it shows the variation of TiO_2 thin films under different heat treatments The transmittance measurement was done in the wavelength settled from $\lambda = 300$ to $\lambda = 500$ nm. This range shows clear variation of red shift indicating decreasing of band gap. The decreasing of transmittance and band gap indicating increase of absorbance that is attributed due increase of particle size upon different heat treatment [17].

3.3 Optical Band Gap

The estimated absorption band edge of the films was computed from the first derivative of optical transmittance as shown in Fig. 3. Te curves between $dT/d\lambda$ and photon energy give a peak that corresponding to the absorption band edge. In this figure the peak position of the curves shifts to lower photon energy wavelengths. This decrease of 0.06 eV band gap is due to increase in particle. Hence, the absorbance below 3.27 eV makes TiO_2 film a righteous choice of light detectors from UV to blue region [18].

3.4 Calculation of Refractive Index from Optical Band Gap

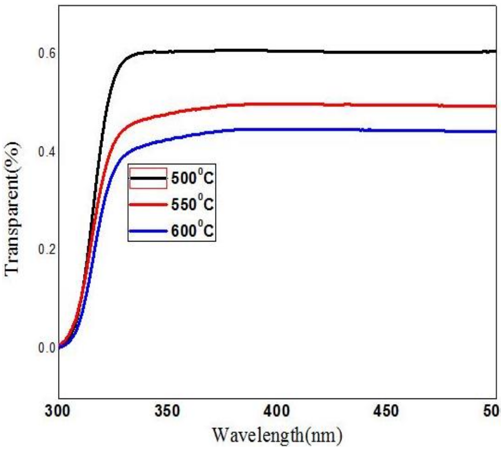

Fig. 2 – The transmittance spectra's of TiO_2 thin films

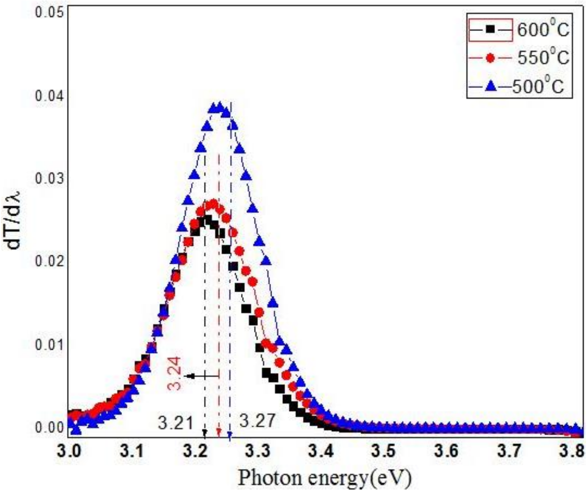

Fig. 3 – First derivative plots of Transmittance of TiO_2 coated films

The refractive index is an important optical parameter to identify the materials behaviour within the light. Reddy et al. has proposed an empirical relation between refractive and band gap for a variety of compounds [19].

$$n = \sqrt{\frac{12.417}{E_g - 0.365}} \tag{1}$$

Equation (1) is the modification of Moss equation [20] with secondary arbitrary constants added in order to improve the results and gives better agreement with the experimental values but can used for low energy band gap values [21]. It's well known that optical absorption is strongly dependent on the electronic transitions over the energy gap E_g. From this point of view, the relation between the refractive index and the optical bandgap has arisen. Generally, the band gap describes the maximum energy at which the transparency of a substance starts to increase. When the energy of light increases toward the optical band gap value, the refraction index should be increased. The theoretical calculations studied for energy base storage and memory devices in order-disorder ferroelectric crystals [22, 23].

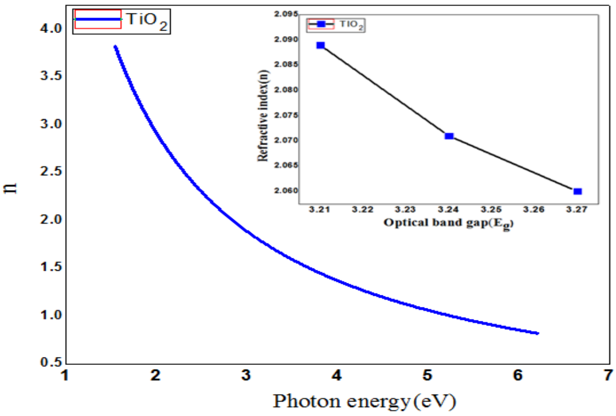

Fig. 4 – Refractive index vs photon energy along with the inset of band gap vs refractive index

TiO_2	Optical band gap(E_g)	Refractive index(n)
500 °C	3.27 eV	2.060
550 °C	3.24 eV	2.071
600 °C	3.21 eV	2.089

4. CONCLUSION

The TiO_2 thin films were prepared by the spray pyrolysis technique and deposited onto ordinary glass substrates. The knowledge of n not listed in the experimental values matches with the calculated by proposed relation may be of great use in potential application regarding opto-electronic properties metal oxide semiconductors, which may be of great use in today semiconductors devices such as lasers, modulators, light-emitting diodes and integrated circuits. A fairly good agreement has been obtained between the calculated and the experimental values. The refractive index is found very sensitive with anhealing, as the decrease of transmission indicates increase in absorbance or refractance of the material.

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Розрахунок показника заломлення з використанням оптичної забороненої зони: тонкі плівки для піролізу розпиленням TiO_2

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Техніка розпилювального піролізу була застосована для осадження широкого діапазону тонких плівок, які використовуються в різних пристроях, таких як сонячні елементи, датчики та твердооксидні паливні елементи. Розпилювальний піроліз є одним із найпоширеніших, недорогих, простих і досить універсальних методів синтезу багатокомпонентних оксидних тонких плівок субмікронних і сферичних люмінесцентних матеріалів. У цій статті тонкі плівки розпиленого піролізу TiO_2 були нанесені на скляні підкладки та витримані при різних температурах, щоб виявити їх оптичні властивості за допомогою УФ-видимої спектроскопії. Показник заломлення (n) тонких плівок TiO_2 як широкого напівпровідника було розраховано з використанням оптичної щілини (E_g). Розраховані значення показника заломлення за новими співвідношеннями були порівняні зі значеннями, повідомленими різними дослідниками; між ними була досягнута чудова угода. Ідентифікація матеріалу була підтверджена методами дифракції рентгенівських променів, і була побудована перша похідна спектрів пропускання, яка відповідно дає значення ширини забороненої зони плівок.

Ключові слова: TiO_2, Розпилювальний піроліз, Заборонена зона, Показник заломлення.