

DEVELOPMENT AND ANALYSIS OF TiO₂ BASED THIN FILM MANUFACTURED BY SOL-GEL METHOD FOR SOLAR CELL APPLICATION

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Abstract— Solar cells have emerged as a promising alternative in the search for clean and renewable energy sources to address the ever-increasing global energy demand. Titanium dioxide (TiO₂) thin films made by the sol-gel process have attracted a lot of interest among the numerous materials used for solar cell applications. The efficiency with which sunlight is absorbed and converted into electricity is essential to the success of solar energy conversion technology. The extraordinary surface-to-volume ratio of thin films, together with their distinctive optical and electrical properties, makes them an attractive platform for collecting solar energy. This paper presents findings from a study into the improvement and analysis of thin films based on TiO₂ that were made using the sol-gel technique for use in solar cells.

Keywords— TiO₂, sol-gel, solar cell, renewable energy, electricity.

I. INTRODUCTION

Searches for sustainable and renewable energy sources have been prompted by rising global energy consumption and environmental concerns. Given its immense potential and relatively small environmental impact, solar energy has emerged as a key role in the shift toward a greener energy landscape. The race is on to create solar cell technologies that are both effective and affordable in this setting. Titanium dioxide (TiO₂) thin films created through the sol-gel process have attracted significant attention due to their distinct optical, electrical, and structural features among the many materials investigated for solar cell for various applications.[1] The development of solar cell technology has allowed for the testing of many different materials in an effort to maximize the efficiency with which they convert energy. The foundation of photovoltaic devices is semiconductors' ability to absorb

photons and create electron-hole pairs. In this regard, TiO₂, a wide-bandgap semiconductor with exceptional electron transport characteristics, represents a promising contender for solar cell applications. Sustainable energy solutions are possible because of its high stability, chemical inertness, and biocompatibility.[2]

Due to their distinct optical and electrical properties, thin films provide a viable platform for solar energy conversion from one form to another form. Improving the efficiency of energy conversion relies on their ability to absorb sunlight with minimal material waste. Carefully designed TiO₂ thin films have a large surface area relative to their volume, which aids in their ability to absorb light and separate charges. Thin films' photovoltaic efficiency can be further improved by engineering them to take on various morphologies, including nanoparticles, nanowires, and nanostructures.[3]

Sol-gel techniques have developed into a flexible way for making specialized thin films. Hydrolysis and condensation of precursor molecules yield a colloidal suspension, or "sol," which, after regulated drying and annealing, crystallizes into a thin film. The film's thickness, composition, porosity, and crystallinity can all affect the material's optoelectronic capabilities; the sol-gel technique makes these variables very controllable. Thin films can be optimized for specific solar cell layouts due to their extraordinary property such as adaptability.[4]

A full suite of characterization methods is required to appreciate the functionality of TiO₂-based thin films. Insights into the film's structure, shape, and optical properties can be gained by the use of techniques including X-ray diffraction, microscopy (SEM and TEM), and spectroscopy (UV-visible and photoluminescence). Methods like impedance spectroscopy are used to investigate electrical properties and reveal charge carrier dynamics and transport mechanisms.[5]

In the present study films made from TiO₂ are studied in more depth than only their elemental characteristics. Researchers are focusing on finding optimal film thicknesses, shapes, and compositions for a wide range of solar cell architectures. With the use of interface engineering and sensitizing dyes or quantum dots, light absorption and electron transmission might be increased. Thin films with improved power conversion efficiency, long-term property stability, and reduced manufacturing costs are being fabricated by researchers utilizing the versatile sol-gel process.

Sol-gel processed thin films based on titanium dioxide are an important step toward efficient and long-lasting solar cell technology, and their development and research is a key part of this road. [6]

This in-depth study aims to optimize the manufacture, structure analysis, optical characterization, and electrical assessment of thin films for use in solar cell applications. Given the increasing demand for energy throughout the globe, the results of this research may help pave the way toward a more sustainable future by significantly enhancing the efficiency with which solar energy is used.[7]

TiO₂ and its variants may be synthesized into thin films using a variety of different synthesis techniques, including sol-gel, micellar, and reversed micellar sol hydro and solvothermal, electrochemical, and others. In addition to (poly) glycols, tetrabutoxytitanium (TBT) is another common precursor. Polyglycols are used as molds for the porous film, determining the pore size. In compared to rutile and brookite, anatase has a narrower band gap, making it the mineral of most interest to researchers. More often than not, however, a mixture of many crystalline forms will emerge. This means that titanium dioxide P25 (Degussa) might have more than a 20% rutile alteration. By adducting TBT with EG, DEG, and TEG, it was found that linear adducts are produced at an equivalent ratio of TBT: TEG, which, after undergoing appropriate heat treatment, produce anatase with a nearly complete stoichiometric composition. [8]

When highly ordered air humidity is present, these adducts in toluene and n-butanol may form gels, as shown in two distinct investigations. Intense heat treatment allows for the production of highly ordered films on a wide range of support materials. TiO₂ films were prepared by, who used a technique that differs from the sol-gel procedure by allowing gelation to occur in true solutions. The use of polyglycols and titanium tetra butoxide (TBT) was noted among the materials put to use. Crystallization and polymorphic transition temperatures have little effects on pore size, which is instead dictated by the specific polyglycols used.[9]

By reacting, TBT and TEG gelled the solution and created TEG TBT-n-butanol, which then solidified into a film during the annealing process. The formation of the adduct with TBT TEG (I), without the polycon densification process, is shown in Figure as one possible explanation.

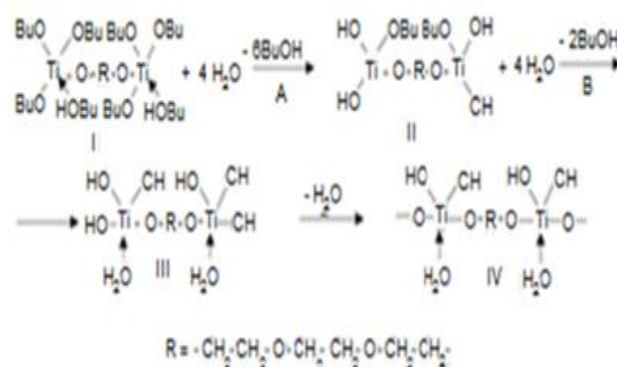


Fig.1: The adduct film-forming process using TBT TEG (I)

Adduct (I) is quickly eliminated in step (A), where six butano molecules and four water molecules connect to create adduct (II). Four water molecules and two butanol molecules are bonded to the adduct (II) in the intermediate stage (B). Condensation under normal circumstances removes the water from the adduct (III), leaving behind the polymeric structure (IV).The focus of this effort is on the gel technique of making TiO₂ thin films from TBT and TEG.

II REVIEW OF LITERATURE

Kim et al. (2022) [10] produced a water-resistant or surface-coatable C-PEG layer onto a glass surface by altering catechol moiety and TiO₂ NP concentrations. The hydrophilic surface made the product self-cleaning.

Lucas et al. (2018) [11] Mortars with self-cleaning capabilities were created by combining PCM microcapsules with TiO₂ nanoparticles.

Zhang et al. (2019) [12] In order to permanently attach nano-TiO₂ to cotton fabric, developed a nano-TiO₂ polyacrylate hybrid dispersion. The finished product's self-cleaning abilities were shown by the natural breakdown of the red wine stain on it when exposed to sunlight.

Peticaet al. (2021) [13]One is that the photocatalytic activity of TiO₂ may produce active components that can react with surface-bound contaminants, leading to their breakdown. The other is that decomposition by-products are easily washed away by rain, keeping the material's surface in pristine condition.

III RESEARCH METHODOLOGY

TBT was used as per protocol. TEG as per the requirements, TU 6-09-2738-9 N-Butyl Alcohol (TU 6-01-5-88).X The samples' -ray diffraction spectra were acquired in step-scan mode using an automated diffractometer DRON 7. With a scanning step of $2\theta = 0.03^\circ$ and an exposure period of 3 s at the spot, the 2θ angle range is from 19 to 90 degrees. The CuK-radiation employed was monochromatic, with a wavelength of $\lambda = 1.5418$. This radiation's spectrum was broken down into its K1 and K2 constituents. "After

approximating the X-ray diffraction profile using the Pseudo-Voigt function, we were able to pinpoint the exact locations of the profile's peaks ($2\theta_{max}$), centre of gravity ($2\theta_{cg}$), line half-width (w), maximum intensity (I_{max}), and background. Then, the intensities were broken down into their integral (I_{int}) and relative (I_{rel}) components.”

A Lambda 950 spectrophotometer with 1 nm resolution captured visible transmission and reflection spectra. At 8 degrees from normal incidence angle, reflectance spectrum was observed. UHV analysis module of Nanofab 25 electron spectroscopy platform captures samples' X-ray photoelectron spectra. Dual-anode Al/Mg X-rays were used to acquire more XPS spectra from the SPECS X-ray Source XR 50. Atomic force microscopy imaged Integra film. The scanning method was tapping.

The research was carried out using a JEOL-2100FX microscope equipped with a 200 keV acceleration voltage. The structural-phase state of the film was determined by analysing electron diffraction patterns acquired in the micro-

diffraction region. Uses Fourier analysis of high-resolution pictures to get estimates of the material's spacing and lattice parameter. The thin films were made using the deep coating technique. TBT and TEG diluted to varying concentrations in n-butyl alcohol (1:1) were utilized. The substrates were sodium glass plates (75 mm x 20 mm x 1 mm). “Following the deep coating process, the samples were air dried for 30 minutes at ambient temperature, followed by 1 hour at 373 K and 4 hours at 723 K. Precursor concentration in n-butyl alcohol, feed solution composition, and deep coating process velocity were all shown to have significant effects on film qualities.”

Table 1: The effect of technical regime factors on the refractive index & film thickness was investigated using integrated optics methods

Samples	Temperature of solution, K	Drying	Calcination temperature, K	Calcination time, h
1	296	+	723	8
2	297	+	723	8
3	298	+	723	8
4	283	+	723	8
5	297	-	753	6
6	296	-	753	6
7	283	-	753	6
8	296	-	873	2
9	283	-	873	2

IV RESULTS

4.1 Examining the influence of process variables and ambient temperature on the effective refractive index & film thickness

$$\frac{2\pi}{\lambda} h(T) \sqrt{n_2^2(T) - n_{effTE}^2(T)} = \text{atan} \left(\frac{\sqrt{n_{effTE}^2(T) - n_1^2}}{\sqrt{n_2^2(T) - n_{effTE}^2(T)}} \right) + \text{atan} \left(\frac{\sqrt{n_{effTE}^2(T) - n_3^2(T)}}{\sqrt{n_2^2(T) - n_{effTE}^2(T)}} \right) + \pi \cdot (\nu - 1);$$

$$\frac{2\pi}{\lambda} h(T) \sqrt{n_2^2(T) - n_{effTM}^2(T)} = \text{atan} \left(\frac{n_2^2(T) \cdot \sqrt{n_{effTM}^2(T) - n_1^2}}{n_1^2 \cdot \sqrt{n_2^2(T) - n_{effTM}^2(T)}} \right) + \text{atan} \left(\frac{n_2^2(T) \cdot \sqrt{n_{effTM}^2(T) - n_3^2(T)}}{n_3^2(T) \cdot \sqrt{n_2^2(T) - n_{effTM}^2(T)}} \right) + \pi \cdot (\nu - 1);$$



Waveguide-optical techniques are one of the most promising approaches to the analysis of the films. The thin film's higher refractive index allows light to go through it and into the substrate. Dispersion calculations for this connection looked like this: where is the radiation source wavelength; n_{eff} is the waveguide mode's effective refractive index; n_1, n_2, n_3 are the refractive indices of air, waveguide film, or substrate; m - number of waveguide modes. "The thickness and refractive index of the film at a fixed temperature may be calculated by experimentally measuring the ERI for two propagating waveguide modes, such as TE1 and TM1. Losses in the film

may also be calculated using the approach given." HeNe laser was utilized as the radiation source, optic wavelength with output and input prism coupler devices as the optical waveguide, TEM as the heater, and a goniometer to determine the waveguide's resonance excitation angles at 293–373 K. The waveguide was excited in the TE1- and TM1-modes. From the gathered data, ERI was determined. A 2105 ERI measurement accuracy was achieved by measuring the waveguide resonance excitation angle with the prism coupler device. Dispersion equation was used to calculate the film's refractive index with thickness temperature dependences.

Table 2: The correlation between temperature and the refractive index

N_2	Temperature
2.12	20
2.13	30
2.6	40
2.5	50
2.4	60
2.017	70
2.016	80
2.09	90
2.07	100

Table 3: The correlation between heat and film thickness

$h, \mu m$	Temperature
0.138	20
0.139	30
0.134	40
1.035	50
0.135	60
0.136	70
0.137	80
0.138	90
0.139	100

It has been seen that the thickness of the film changes significantly as the temperature increases within the considered range, and that the film's refractive index decreases as the temperature increases, indicating that the film has a negative TO C with a value of $\beta - 3104 \text{ }^\circ\text{C}^{-1}$. Sol-gel films have a TOC similar to this value.

4.2 Spectral analysis of film transmission and reflection

Hydrolysis in the film results in an oligomer with a linear structure, hence the film is likely to be anisotropic. Anisotropy strength is proportional to crystallites' mutual orientation, size, and form. Transmission and reflection spectra of the films were analysed to provide light on the films' potential anisotropy characteristic.

It is clear from the preceding analysis that TiO2 films may exhibit substantial birefringence over the whole visible

spectrum. "The birefringence, measured as the difference between the refractive indices of two polarizations of light, is about equal to 0.1. In comparison to other known nonlinear optical materials this result is on par." Transmission electron microscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy were used to examine the films' structure and morphology. "Cell characteristics may be determined by analysing the X-ray diffraction data of the breakdown products of the adduct TBT-TEGs after heat treatment at 723 K." After 5 hours of heating at 723 K, the samples will have formed a crystalline coating in anatase form. As can be observed, there is a strong agreement between experimental and theoretical data.

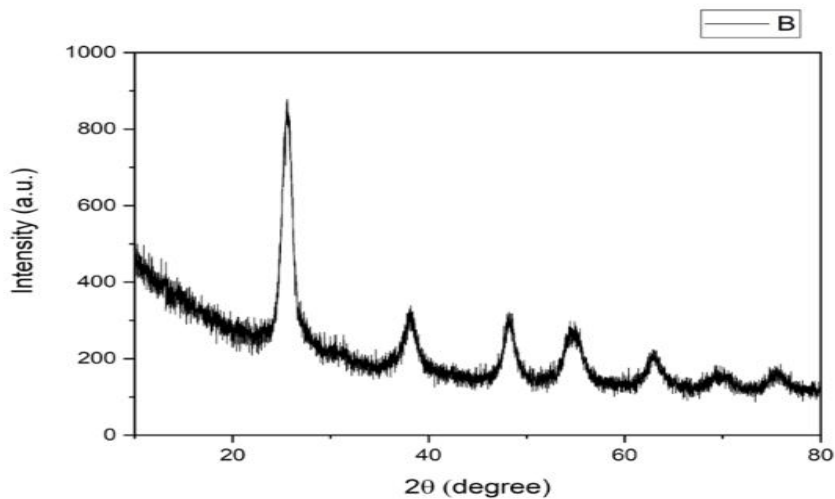


Fig. 2: XRD result of TiO₂ between Intensity and 2θ

Samples produced at low calcination temperatures showed big particles with a maximum particle size of 3-5 μm and poor dispersions, as evidenced in SEM pictures. Increased calcination temperature to 400 or 500 °C reduced particle size to sub 1 μm with good dispersions, showing stable TiO₂ grains. Grain size increased to 1-2 μm after 600 °C calcination. Anatase TiO₂ has 0.352 nm interplanar spacing on its (101) face, as shown in magnified photographs. As a result, what seems like micron-sized particles in SEM pictures are really just aggregates of nano-sized particles.

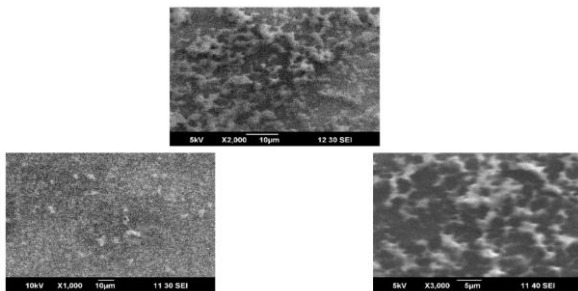


Fig. 3: SEM image of TiO₂ thin film

V. DISCUSSIONS

The transparent TiO₂ thin films that were successfully fabricated using the sol-gel process demonstrate the feasibility of consistent material deposition. Assuring uniform light absorption and charge separation across the film is critical for solar cell applications. The films' transparency is an advantageous feature since it allows for more light penetration and use inside the solar cell device. It is interesting to notice that the created TiO₂ thin films have a negative thermo-optic coefficient. The fact that this coefficient changes with changes in other process factors like the component ratio of the solution indicates that the optical characteristics of the film are affected by the circumstances under which it was fabricated.

The film's thermal stability and its sensitivity to temperature fluctuations may be affected by how well this coefficient is understood and controlled, which in turn may affect the film's optical performance under varying circumstances of use. Understanding the correlation between film thickness and water content, as shown in this work, is essential for achieving optimal film characteristics. Reduced film thickness variation in comparison to the sol-gel technique highlights the importance of water content in shaping the material's morphology. The film's performance and durability may be affected by the time-to-time variation in thickness, and the reduced water content in the pores of the film adds to this.[14] TiO₂ films were employed as a self-sterilization surface in experiments [15], where they killed several bacteria following irradiation with UV light by producing reactive oxygen species. The formation of nanopores on the surface of TiO₂ films was reported as a novel method to improve the films' antibacterial properties. [16] "Researchers analyzed the bactericidal effects of TiO₂ films on both Gram-positive and Gram-negative bacteria and found that the modified surface possesses significantly higher antibacterial activity as compared to the conventional TiO₂ surface film. [17] This is likely due to the increased surface area of the modified surface and changes in the microstructure of TiO₂ induced by laser exposure." [18] Atomic force microscopy analysis of the bacteria after incubation revealed morphological alterations indicative of cell wall damage from UV and/or ROS exposure. This damage may be repaired by annealing the TiO₂ at temperatures over 400 °C, restoring its bactericidal action.[19] Titanium isopropoxide was used to create TiO₂ films on silica-coated soda-lime glass plates, and its photokilling activity against E. coli cells was examined by Sunada and colleagues [20]. The scientists discovered that the photocatalytic process negatively impacted cell viability by inflicting damage on the cell's exterior. TiO₂ film

photocatalyst, they reasoned, breaks down E. coli cell wall lipopolysaccharide.[21]

TiO₂ films on glass substrate were created [22] using tetrabutyltitan as the TiO₂ precursor. "TiO₂ films were tested for their bactericidal efficacy against Gram-negative and Gram-positive bacteria when exposed to UV irradiation at a wavelength of 380 nm." A 12-minute exposure to UV radiation reduced the viability of *S. aureus*, *S. epidermidis*, and *E. coli* by 29, 45, and 47%, respectively. [23]

The scientists also noted that the photoinduced bactericidal activity of the TiO₂ was lost after a single application, but that it could be re-established by annealing the material at temperatures over 400 degrees Celsius.[24] Design, characterization, and antibacterial assessment of TiO₂ & TiO₂-doped films against *E. coli* are shown. The authors postulate that the films' primary bactericidal activity is the disruption of bacterial cell walls.[25]

VI. CONCLUSIONS

Titanium dioxide films that are both clear and homogenous were created using the gel approach in this study. Further, the ratio of the components of the solution, as well as other technical process factors, affect the value of the negative thermo-optic coefficient of the manufactured films. The quantity of water contained in the film's pores is lower, resulting in a less dramatic change in film thickness compared to the sol-gel process. Evidence of anisotropy in a TiO₂-based film suggests it might be employed in a variety of IO setups. As shown, the films' porous nature enables doping with chemicals, which in turn enables the fabrication of IO active devices like lasers, amplifiers, etc.

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