Study of the Relationships Between Optical and Physical Properties for Nanostructure TiO$_2$ Thin Film

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Abstract

Pulsed Laser Deposition (PLD) technique was performed to deposit the pure Titanium oxide (TiO\textsubscript{2}) nanoparticles on the glass substrate of temp. (100 - 400°C), using the doubled frequency of Nd: YAG laser wavelength of 532nm at (10) Hz rate, 10 nanosecond duration pulses and a constant laser energy 800 mJ. The optical measurements obtained by UV-Vis transmittance on deposited TiO\textsubscript{2} films indicate the highest transparency in the visible wavelength region with an average transmittance of 80%. Estimated the relationship between the refractive index of TiO\textsubscript{2} thin films with substrate temperature was n = 2.49 at 400 oC. Moreover, the calculated empirical relation between the energy gap and refractive index have similar to the work results.

1. Introduction

The most common material for generations as solar cell as nanostructure and high storage like nanobatteries selected according to durable, low-cost, and eco-friendly depends on the crystal structure features of the materials [1–5]. Titanium dioxide TiO\textsubscript{2} (Titania) is one of the most inexpensive, non-toxic, environmentally friendly and highly efficient semiconductor materials for many applications, including energy and environmental due to its strong oxidizing ability, high resistance to photochemical corrosion and high efficiency in decomposing pollutants that accumulate on surfaces Such as roofs of buildings or windows and surfaces of olfactory cells that affect their efficiency in the future. Nanotechnology, especially using nanostructures such as titanium, provides self-cleaning, transparent and highly conductive surfaces [1, 2]. TiO\textsubscript{2} has three crystalline structures: brookite, anatase, and rutile [7]. In addition, particle size plays an important role in nanocrystals for the functioning of solar cells on TiO\textsubscript{2}. The nanostructured surfaces provide a large surface area, which allows increasing the activity of high absorption of sunlight effects on the recombination dynamics e\textsubscript{-}/h\textsuperscript{+}, adsorption amount of reaction types and adsorption rate [5-6]. TiO\textsubscript{2}, WO\textsubscript{3} and ZnO have received wide attention lately due to its unique and important properties, Making it great and wide applications in various fields. Suitable for use in photovoltaic elements, dielectrics, capacitors, or gates in photovoltaic solar cells, microelectronic devices, biosensors, position sensor anti-reflection coatings, photonic crystal, and photo guides [3], metal-based devices, nano random lasers, and other similar applications [7–11]. Due to the particular qualities of TiO\textsubscript{2} films with distinct crystal structure, orientation, or shape, controlling TiO\textsubscript{2} films structure during growth is essential. TiO\textsubscript{2} films have been created using a variety of techniques, including rotary coating, pulsed laser deposition, anodizing, oxygen plasma-assisted molecular beam amplification. PLD technology, for example, has been extensively utilized to build oxide films because it enables the stoichiometry of the composite material to be achieved. Because the Si substrate is extensively utilized in semiconductor manufacturing, the development of TiO\textsubscript{2} films on Si by PLD has piqued the curiosity of many researchers and industry professionals’ curiosity. TiO\textsubscript{2} nanostructure is a one-of-a-kind material with a greater bandgap of 3.2 eV than rutile, with a bandgap of 3 eV. Because of their various features, such as high refractive index, broad bandgap, and resilience to physical and chemical effects [11, 12], anatase and rutile bulk offer potential for use in sensing applications[5].
The electric symmetry in solar cells is used to transport electrons away from the proximity of their initial state, so preventing the relaxation of the cell’s electrochemical properties. This results in an energy transfer to excited electrons from photons. The energy transferred to excited electrons increases potential difference, which may be utilized to drive current via an external circuit [13–25].

In the present study, the pure Titanium oxide (TiO₂) nanostructures on glass substrate were synthesized by pulsed laser deposition (PLD) at different temperatures was prepared. Also, evaluation of the relationship between optical and physical properties (optical constants, energy band gap, density and porosity, and refractive index,) of TiO₂ thin films have been estimated.

2. Experimental Work

2.1 Target Preparation

The substrate raises the substrate temperature to 600°C by heater 650W halogen lamp. The temperature was measured of the glass by a K-type thermocouple. The glass dimensions slide each 3 x 2 cm² area and clean by alcohol using ultrasonic waves supply by co. Cerry PUL 125 device for 15 minutes to remove the contamination and dust from their surfaces. Figure 1 depicts an optical picture of a TiO₂ film that has been deposited on glass via PLD. Figure 1 is a schematic representation of the whole PLD system, including its components in figure 2.

2.2 Deposition of TiO₂ Thin Film by PLD

The TiO₂ films were prepared under vacuum (10-3 Torr) at laser power of 800 mJ with different temperatures ranging from (100-400) °C by using two background gases, active gas and inert gas, in order to achieve the desired properties (O₂&Ar). The configuration of the substrate mounts, and objective inside the chamber in relation to the laser beam is seen in Figure 2. Q-switching Nd:YAG SHG laser beam focused on the surface at a 45-degree angle to the surface of the target.

2.3 Characterization:

A Shimadzu dual-beam UV-VIS spectrophotometer (SP8001) was used to measure the optical properties of the TiO₂ films were deposited on glass (transmittance and absorption) under various conditions. For each scan, a background correction was taken. The absorption coefficients for films at different wavelengths can be calculated using the transmittance and absorption data. Which was used to define the bandgap, for example. The average thickness of the films prepared using the optical method (laser light interference) was measured at about 150 nm.

3. Results And Discussion

3.1 Transmission and Absorption
According to the results of the UV-Vis spectrophotometer measurements of TiO2 films optical transmittance on the glass formed by PLD, the transmittance is highly dependent on the temperature of the substrate, as seen in figure 3. It is average transmittance of the TiO2 film exceeded 85 percent in the infrared region of the spectrum, which is where it was tested. This demonstrates that TiO2 film may be used as the material of a solar cell after being recycled. When the temperature of the substrate is raised, it is seen that there is a modest reduction in the optical transmittance of all of the studied films. The optical absorption are located at (0.55, 0.65, 0.75, 0.85) %, which corresponds to temperatures of (300, 200, 400, and 100) °C, respectively, and are measured in per cent.

Figure 4 Enhancement It can be seen from the transmission findings that absorbance is highly dependent on the ambient temperature. Further investigation showed that the TiO2 absorbance coatings rise with rising substrate temperature, except when the temperature is 400 degrees Celsius or below.

3.2 Refractive Index (n):

From equation one and figure 5, the refractive index is measured by using equation 1. The shape of the curves with a wavelength of the refractive index as a function of wavelength of TiO2 films in figure 5 are the same curves as transmittance curves because both relations are increased with high temperatures, as shown in figure 5. The index of refractive for TiO2 is rising with high temperatures. From figure conclude the refractive index at wavelength $\lambda = 550$ nm is equal (2.11, 2.88, 2.80 and 2.49) of the films with substrate temperatures of (100, 200, 300 and 400) °C respectively, coincident results with reference [27].

According to [28], the enhanced results may contribute to the rise in packing change and density in the crystal structure, and the increase in results has been linked to the promotion of crystal growth.

$$n = \frac{1 + \sqrt{R}}{1 - \sqrt{R}} \quad \ldots \ldots \ldots (1)$$

The conclusion that various of the refractive index with a wavelength of the deposited TiO2 / glass is explained in figure 5. TiO2 refractive index was found to be $n = 2.49$ at the $\lambda = 550$ nm at 400 °C agreement this result with reference [27] for TiO2 films by PLD technique.

The relation between the refractive index of TiO2 film with substrate temperature is illustrated as shown in figure 6.

To conclude the TiO2 film density ($\rho$) in the unit gram/cm$^3$, can be used the following expression ($\rho = (n_f - 0.91933) / 0.42751$) ....(2) where the $n_f$ is the refractive index of the TiO2, films. This expression can conclude the relationship between substrate temperatures and TiO2 film density explained in Figure 7.

The density of the deposited TiO2 film is calculated at $\lambda = 550$ nm by the above expression and is equal to be $\rho = 3.6881$ g/cm$^3$ [27–29].
4. Conclusion

The current study has created crystalline TiO2 thin films that have been effectively deposited onto a glass substrate using PLD. Because of their excellent transmittance, these thin films have the potential to be used as windows in solar cell manufacturing. The optimal substrate temperature is equivalent to 400 degrees Celsius, and the optimum transmittance of TiO2 film is around (80%) for thickness 150nm. The link between the temperature of the substrate and the refractive index of TiO2 thin films was attempted to be calculated. Increasing the substrate temperature to 400 degrees Celsius results in a rise in refractive index to n = 2.49. Conclusion: At 400 degrees Celsius, the density of the formed TiO2 sheets is determined to be 3.6881 grammes per cubic centimetre, which is expected to be homogeneous.

Declarations

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**Figures**

![TiO\textsubscript{2}/Glass](TiO\textsubscript{2}/Glass.png)

![TiO\textsubscript{2}/Si](TiO\textsubscript{2}/Si.png)
Figure 1

Optical photograph of TiO$_2$ film deposited by PLD on glass.

Figure 2

Photograph of Pulsed laser deposition (PLD) system.
Figure 3

Illustrated the relationship between transmission vis of wavelength for TiO$_2$/ glass at temperatures between (100 – 400 °C).
Figure 4

illustrated the relationship between absorption spectra of the TiO$_2$/ glass films at variance temperatures with range values (100 – 400 °C) & laser energy at 800 mJ.

Figure 5

Refractive index as a function of wavelength for the different temperatures of TiO$_2$ thin films.

Figure 6

Estimated the relationship between refractive index & substrate temperature of TiO$_2$ thin films.

Figure 7

Explain the density $\rho$ verse of substrate temperature of TiO$_2$ thin films.