Study on the optical and structure properties of TiO$_2$ for different thickness prepared by spray pyrolysis

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Abstract. Thin films TiO$_2$ prepared by thermal pyrolysis technique were examined for different thickness (75 to 375 step 75 nm). The results showed that the best transfer was 75 nm (89%), the allowable direct transfer calculation is equal to (3.4-3.68 eV).

Keywords: optical properties of TiO$_2$, TiO$_2$, spray pyrolysis.

1. Introduction: TiO$_2$ films have been extensively studied because of their important catalytic properties of images. TiO$_2$ films contain many different application areas, such as: optical stimulation, gas sensing, anti-reflective coating, antibacterial and optical coating, etc. TiO$_2$ is a light-sensitive semiconductor. When lighting the power lamp higher than the band gap, transmission between bands can occur and generate electron hole pairs. Some of these light-emitting pairs separate the charge and spread to the surface of TiO$_2$, react with air or water and eventually generate OH, anionic roots, which attack the organic compounds absorbed on TiO$_2$ surface and remove them by switching to CO$_2$ and H$_2$O. The surface of TiO$_2$ thus becomes strongly oxidized and can act as a photocatalyst as shown in fig.1 [1-4].

![Fig. 1: The crystal structures of (TiO$_2$) [6].](image)

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The physical and chemical methods used for the preparation of titanium dioxide films (physical methods: magnetron, constant current or radio frequency, electronic beam evaporation, PVD, thermal evaporation), chemical methods: sol-gel, anodic oxidation, pyrolysis For spray, chemical vapor deposition (CVD)), etc.

2. **Experimental work:** The diagram below shows the direction of experimental work

![Diagram showing experimental work]

**Fig.2:** The diagram shows the direction of experimental work

Sedimentation method involves dissolving aqueous solution of titanium chloride. The spray solution is sprayed from different molars (different thicknesses, 75 to 375 step 75 nm). On heated substrates (± 500 °C). The compressed air is used as a gas carrier and fed with the solution in the spray nozzle at pre-set pressure.
Thin films of (TiO₂) prepared from titanium chloride (TiCl₃) diluted with distilled water, (TiCl₃) is a liquid material which has a violet color and its molecular weight (154.26 ml/mol.). For calculating mass of (TiCl₃) in the current experiment we use the following equation [8]:

\[ M = \frac{W_t}{M_{wt} \times \frac{V}{1000}} \quad (1) \]

When (M) and (Wt) are a concentration of molarities and weight of (TiCl₃) respectively, also, (Mwt) is molecular weight of (TiCl₃) and V is volume of distilled water. TiO₂ prepared as a solution from equation [7]:

\[ 2TiCl₃ + H₂O \rightarrow Ti(OH)₂Cl₂ + TiCl₄ \]

\[ Ti(OH)₂Cl₂ \rightarrow \downarrow TiO₂ + ↑ 2HCl \]

3. Result and Discussion: The XRD test of films deposited on glass substrate indicated that the films had polycrystalline and anatase titanium dioxide [9].
Figure 5 shows the permeability spectrum of TiO2 films of different thickness (75 to 375 step 75 nm). Maximum permeability (75 nm) was observed for wavelength (300-900 nm). However, permeability decreases when fish increase [9]. This behavior is due to an increase in the number of atoms in fish, increasing the number of collisions between accident atoms, which in turn increases absorption and reduces permeability [10].

The Absorption of TiO2 films as a function of thickness were shown in Fig. (6), the absorption increases with increasing the thickness [11].
Reflectance is a ratio of the reflected and incident intensity rays. [7]. Reflectance is calculated from spectrum of absorbance and transmittance for all prepared thin films. We observed that reflectance have high value which decreasing with wavelength increasing for all films, as in figure (7).

\[ \text{Absorption coefficient is calculated by using equation:} \]
\[ \alpha = \left( \frac{2.303 A}{t} \right) \] [12]

When absorption coefficient ($\alpha$), thickness ($t$), and absorbance ($A$).

($\alpha$) As a function of wavelength and photon energy receptively can be seen in Figure (8), ($\alpha$) is increasing with thickness increase as a function of photon energy.

\[ K_{\alpha} = \alpha \frac{\lambda}{4\pi} \]

Where $\lambda$ is the wavelength of incident photon rays.
Figure (9) illustrates \((K_0)\) as a function of wavelength for \((\text{TiO}_2)\) films. The excitation factor behaves in the same behavior as \((\alpha)\) because it is associated with a previous relationship, and the extinction coefficient decreases with increasing thickness

![Figure 9: Excitation coefficient as a function of wavelength.](image)

Refractive index is measured by using relation [14]:

\[
n = \frac{1 + \sqrt{R}}{1 - \sqrt{R}}
\]

It has been shown in figures (10) as a function of wavelength of \((\text{TiO}_2)\) films. The shape of the curve with wavelength is the same curve \(R\) curve because the relation between them is increased with photon energy increasing and then decreases, \(R\) index increases with thickness increasing.

![Figure 10: Refractive index as function of wavelength for different thickness of \(\text{TiO}_2\) thin films.](image)
The energy gap for all films can be calculated from equations [16]:

\[(\alpha h \nu)^2 = B2 (h \nu - E_{gopt})\]

**Table 1:** Direct energy gap for different thickness of TiO₂ thin films.

| Thickness (nm.) | Eg (eV) |
|-----------------|---------|
| 75              | 3.680   |
| 150             | 3.62    |
| 225             | 3.6     |
| 300             | 3.48    |
| 375             | 3.4     |

**Fig. 11:** Allowed direct electronic transitions of TiO₂ thin films
4. **Conclusions:** From (X-ray diffraction) investigation observed crystalline structure of (TiO2) film has (polycrystalline) structure and synthesis (tetragonal), the best transmittance of (TiO2) film is (89%) for thickness (75nm.), within range (400-900nm.), the film is good to be window of silicon solar cell. But (A) is high at short wavelength, therefore; the film is good to be detector within ultra-violet region range. (n ) of films are in the range of (4.6-6.7). This means that the film is good to be antireflection coating. This converts to a large probability that direct electronic transition will happen. Energy gap for allowed direct transition has been calculated and it is equal to (3.4- 3.68 eV).

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