# Optical properties of $TiO_2$ thin films prepared by reactive d.c. magnetron sputtering

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**Abstract**

$TiO_2$ thin films were deposited by reactive d.c magnetron sputtering method on a glass substrate with various ratio of gas flow (Oxygen /Argon) (50/50, 100/50 and 150/50) at substrate temperature 573K. It can be observe that the optical energy gap of $TiO_2$ thin films dependent on the ratio of gas flow (oxygen/argon), it varies between (3.45eV-3.57eV) also it is seen that the optical constants (α, n, K, $\varepsilon_r$ and $\varepsilon_i$ ) has been varied with the change of the ratio of gas flow (Oxygen /Argon).

**Key words**
*Optical properties,*
*Reactive d.c. magnetron,*
*$TiO_2$ thin films.*

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## الخصائص البصرية لاغشية $TiO_2$ المرسب بطريقة الترذيذ المغناطيسي

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**الخلاصة**

رسبت اغشية $Tio_2$ بأستخدام طريقة الترذيذ المغناطيسي على ركائز من الزجاجية بنسبة مختلفة من تدفق غازات كل من (الاكسجين / الارجون) (50/150 و 50/100 و50/50) وفي نفس درجة حرارة الركيزة 573K. درست الخصائص البصرية لاغشية $TiO_2$ وتم تحليلها ووجد ان فجوة الطاقة الضوئية لاغشية ال $TiO_2$ تعتمد على نسبة تدفق الغاز ( الاكسجين / الارجون ) ، حيث تتغاير ما بين (3.45eV-3.57eV) وكذلك وجد ان الخصائص البصرية (α , $\varepsilon_i$, $\varepsilon_r$, K , n) تتغير مع تغير نسبة تدفق الغازات ( الاكسجين / الارجون ).

## Introduction

Titanium dioxide is considered as one of the most important materials from the point of view of both fundamental properties and applications because of their desirable properties, such as good transmission in the visible and near infrared regions, good adhesion, and high stability against mechanical abrasion, chemical attack, and high temperatures [1, 2].

The goal of this research is control the structural and optical properties of the thin films prepared by d.c magnetron sputtering with varies ratio of gas flow (Oxygen /Argon) at fixed temperature substrate .

Titanium dioxide can exist as an amorphous layer and also in three crystalline phases:- anatase (tetragonal), rutile (tetragonal) and brookite (orthorhombic) [3].

Many deposition methods can be used to prepare titanium oxides films: arc ion plating [4] sputtering [5], pulsed laser deposition (PLD)[4], sol-gel method [6]. Here we investigate the influence of $O_2$/Ar gas flow ratio during the preparation of the Titanium oxide films on their structural and morphological properties and then reports on the analysis of the samples by use of X-ray diffraction (XRD) and scanning electron microscopy (SEM).

## Experimental Techniques

$TiO_2$ thin films were prepared by built reactive d.c magnetron sputtering; a circular magnetron with 60mm diameter was used as cathode. The discharge characteristics have been controlled using variable dc power supply (5KVand 500 mA). Pure Titanium (99.995) of 100 mm diameter and 2mm thickness has been used as a sputtering target. Pure Argon and Oxygen were used as the sputtering and reactive gases respectively. The distance between the target and the glass substrate was 50mm. The substrate temperature was controlled using a quartz halogen lamp. The sputtering pressure kept at $6*10^{-1}$ mbar and the set up of the reactive d.c. magnetron sputtering system is shown in Fig1.

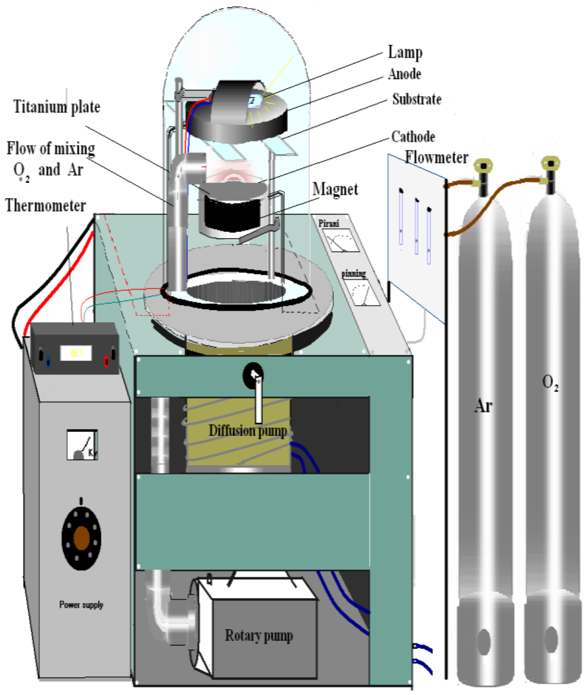


*Fig. 1: Reactive d.c magnetron sputtering*

## Results and Discussion

Fig.2 shows the XRD pattern for $TiO_2$ thin film deposited by reactive d.c magnetron sputtering method on a glass substrate with various ratio of gas flow (Oxygen /Argon) (a) 50/50, (b) 100/50 and (c) 150/50. The XRD patterns show the mixed phases brookite, anatase and rutile. The first peak denoted the anatase or brookite phases, second phase is rutile, third and fourth peaks are brookite and fifth peak is anatase or rutile. We should point out that the changes only in the width and intensity of the peaks as shown in Fig.2 (a, b and c). The interpretation of this result is due to increase in the grain size of $TiO_2$ thin films as the Oxygen/ Argon ratio increases (see Table 1).

Table1 shows a comparison between the experimental and standard value of $d_{hkl}$ for the peaks that showed in XRD patterns. The particle (G) size is described by Scherrer's formula [7]:

$$G = \frac{0.89\,\lambda}{\Delta(2\theta).\cos(\theta)}$$

From the table, we can see that all films have overlapping for all $TiO_2$ phases Brookite, Anatas and Rutile and the particle size increases with increasing of the oxygen flow rate.

Using scan electron microscope (SEM) we can see the surface structure of $TiO_2$ thin films prepared at 50, 100, and 150 sccm (stander cubic centimeter per minute) Oxygen flow rates with constant Argon flow (50 sccm) as shown in Fig.3 (a, b, and c). The grain size has smaller diameters and better smoothness because the Oxygen flow is lower and grain size is enlarged when the Oxygen flow increases.

The optical transmittances of the films were recorded as a function of wavelength range 200-1100 nm using UV/VIS-spectrophotometer model(2601). Fig.4 shows the transmission spectra for $TiO_2$ thin films formed at various oxygen flow 50, 100 and 150 sccm with mixture constant flow argon 50 sccm. It can be observed that the transmission coefficient has a high value in the visible region and increase with increasing of ratio of oxygen. The optical transmission in the wavelength 400nm increases from 45% to53% with increasing oxygen flow from 50 to150 sccm. The reason may be due to the changed in surface morphology of the thin films. This result has been similar to Stamate [8] and the light loss by scattering of defect centers decreased which an increase in the optical transmission.

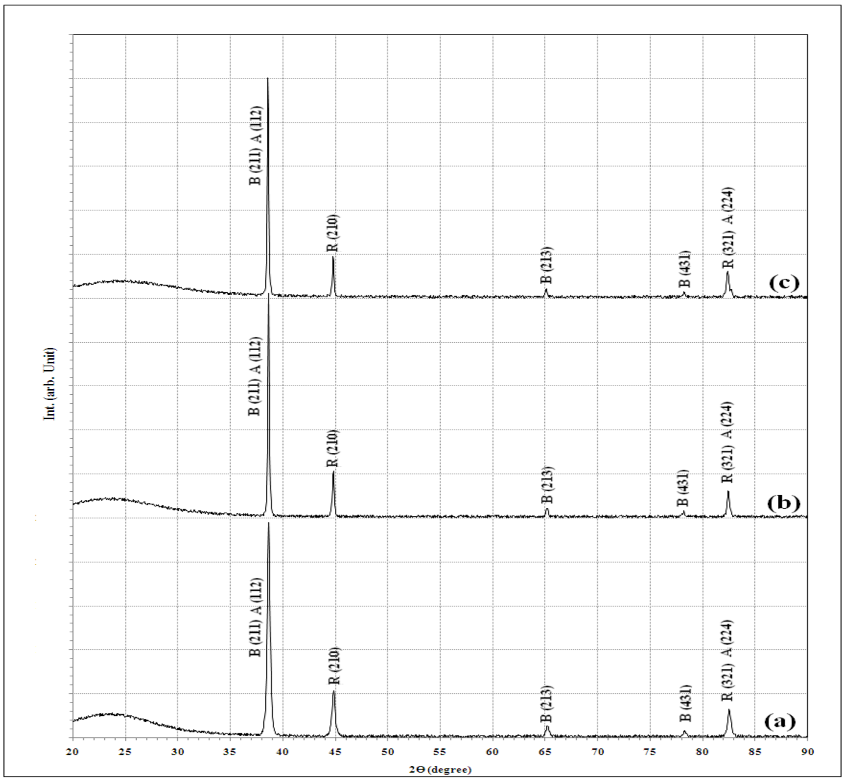


***Fig. 2: XRD Pattern For $TiO_2$ thin film deposited at various ratio of gas flow (Oxygen /Argon) (a) 50/50, (b) 100/50 and (c) 150/50***

***Table1: Comparison between the Exp. and Std. value of $d_{hkl}$ for the peaks showed in XRD and the grain size and the identically with which phases.***

| gas ratio | 2θ (degree) | FWHM | Int arb. unit | $d_{hkl}$ Exp.(Å) | G.S (Å) | $d_{hkl}$ Std.(Å) | phase | hkl |
|---|---|---|---|---|---|---|---|---|
| 50/50 | 38.626 | 0.306 | 2464.8 | 2.329 | 259.143 | 2.332 | Brookite | (211) |
| | | | | | | 2.332 | Anatase | (112) |
| | 44.817 | 0.329 | 535.1 | 2.021 | 246.036 | 2.054 | Rutile | (210) |
| | 65.189 | 0.349 | 113.5 | 1.430 | 254.737 | 1.433 | Brookite | (213) |
| | 78.287 | 0.350 | 56.8 | 1.220 | 275.627 | 1.220 | Brookite | (431) |
| | 82.513 | 0.353 | 308.1 | 1.168 | 281.927 | 1.170 | Rutile | (321) |
| | | | | | | 1.166 | Anatase | (224) |
| 100/50 | 38.621 | 0.190 | 2652.3 | 2.329 | 417.585 | 2.332 | Brookite | (211) |
| | | | | | | 2.332 | Anatase | (112) |
| | 44.784 | 0.200 | 533.6 | 2.022 | 404.682 | 2.054 | Rutile | (210) |
| | 65.164 | 0.222 | 97.0 | 1.430 | 400.007 | 1.433 | Brookite | (213) |
| | 78.175 | 0.250 | 56.6 | 1.222 | 385.572 | 1.220 | Brookite | (431) |
| | 82.424 | 0.270 | 291.0 | 1.169 | 368.344 | 1.170 | Rutile | (321) |
| | | | | | | 1.166 | Anatase | (224) |
| 150/50 | 38.561 | 0.165 | 2500.2 | 2.333 | 480.497 | 2.332 | Brookite | (211) |
| | | | | | | 2.332 | Anatase | (112) |
| | 44.768 | 0.170 | 469.0 | 2.023 | 476.070 | 2.054 | Rutile | (210) |
| | 65.077 | 0.190 | 88.9 | 1.432 | 467.150 | 1.433 | Brookite | (213) |
| | 78.238 | 0.220 | 56.6 | 1.221 | 438.346 | 1.220 | Brookite | (431) |
| | 82.362 | 0.300 | 291.1 | 1.170 | 331.353 | 1.170 | Rutile | (321) |
| | | | | | | 1.166 | Anatase | (224) |

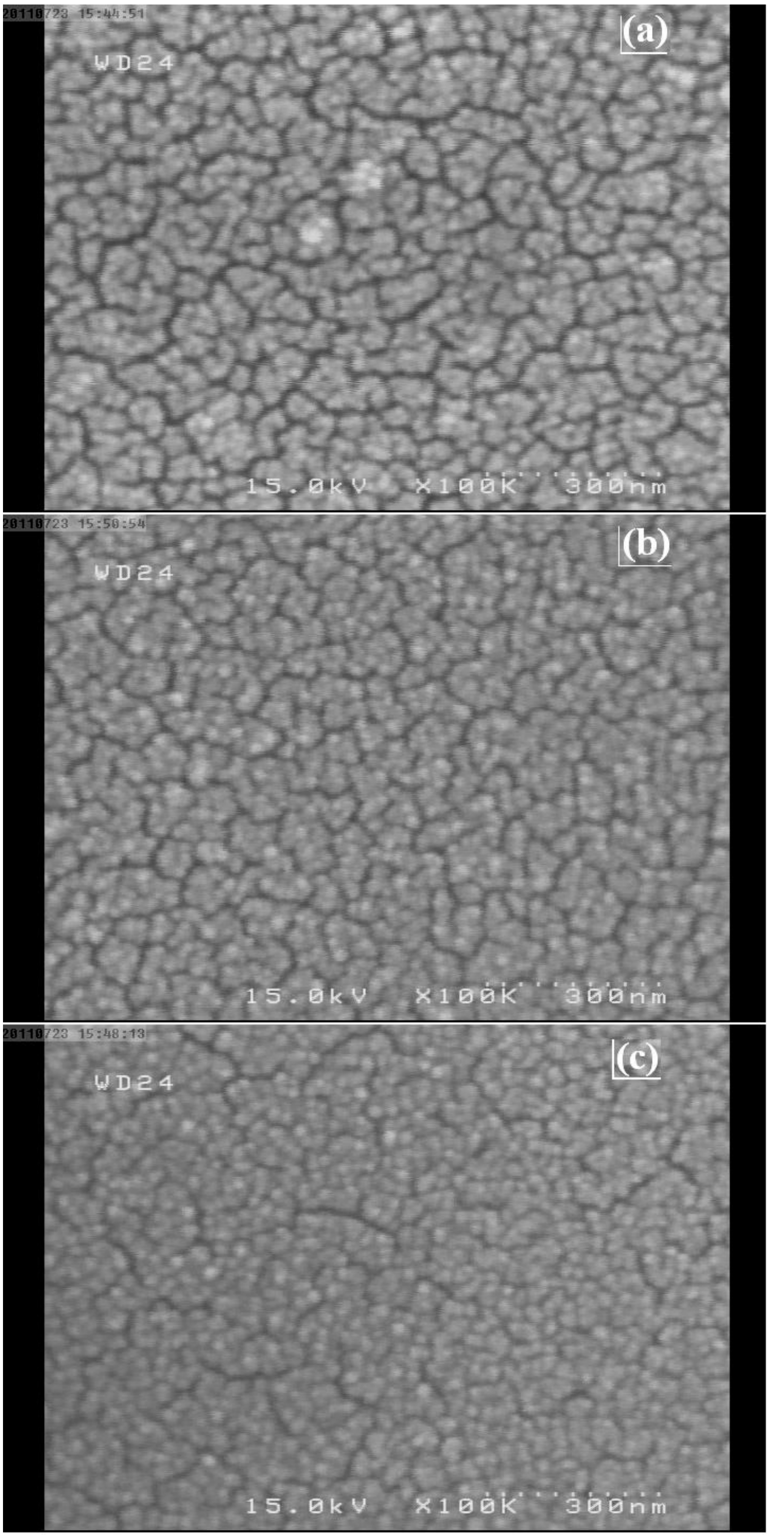


***Fig 3: SEM For $TiO_2$ thin film deposited at various ratio of gas flow (Oxygen /Argon) (a) 50/50, (b) 100/50 and (c) 150/50***

Fig.5 shows the optical absorption coefficient (α) as a function of the wave length for $TiO_2$ thin films at different ratio of oxygen flow. It is cleaned the (α) decreases with the increasing of oxygen flow. From Fig.6, the extinction coefficient (K) is also found to decrease when the flow of oxygen increases. In the visible region, all the films exhibit very low extinction coefficient.

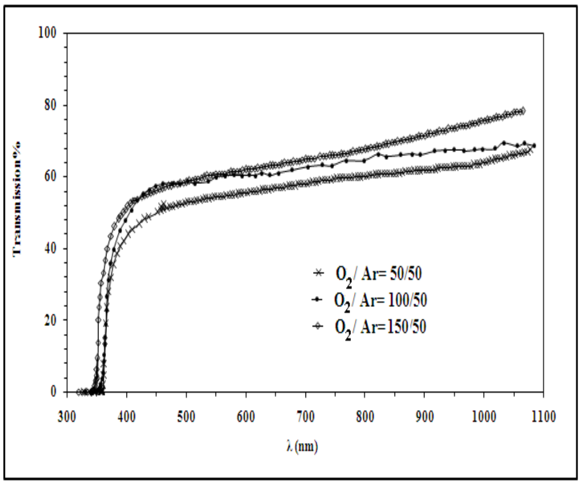


***Fig.4: Optical transmittance spectra of $TiO_2$ films vs. wavelength formed at various ratio of gas flow (Oxygen /Argon)***

The refractive index (n) decreases from 2.69 to 2.28 at 400nm wavelength and the flow oxygen increases from 50 to 150 sccm as shown in Fig.7. The refractive index is in good agreement with Suhai [9] which prepared $TiO_2$ films using sputtering technology.

Also, the dielectric loss increase from 0.22 to 0.27 at 400nm wavelength when the flow of oxygen increase 50 to 150 sccm as shown in Fig.8, while the real part of dielectric constant increases from 3 to 6.4 at 400nm wavelength when the flow of oxygen increases 50 to 150 sccm as shown in Fig.9, and also the real and imaginary part of dielectric constant decreases in visible wavelength.

The optical bandgap Eg was evaluated from the plots of. $(\alpha h\upsilon)^2$ vs. photon energy hυ. The optical bandgap depends on the oxygen flow Fig.10, Eg increases from 3.45 eV to 3.57 eV with increasing of the oxygen flow from 50 to 150 sccm. The result of Eg is in good agreement with the films deposited by magnetron sputtering Meng[10].

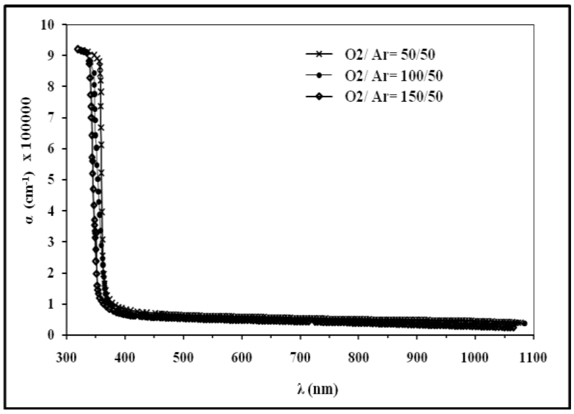


***Fig.5: Optical absorption coefficient (α) of $TiO_2$ films vs. wavelenght formed at various ratio of gas flow (Oxygen /Argon)***

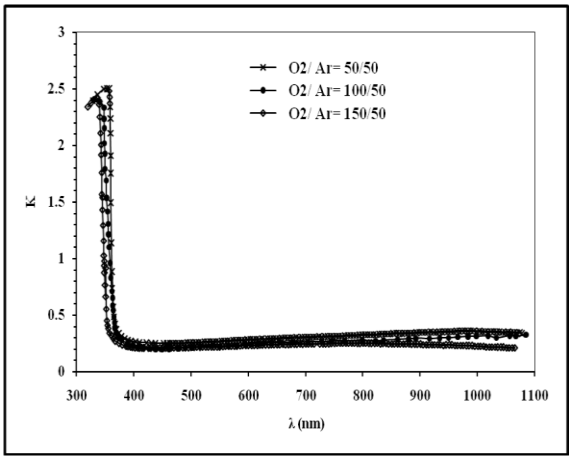


***Fig.6: Extinction coefficient (K) of $TiO_2$ vs. wavelenght films formed at various ratio of gas flow (Oxygen /Argon)***

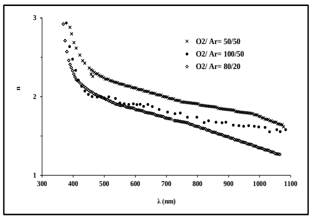

***Fig.7: Refractive index (n) of $TiO_2$ films vs. wavelenght formed at various ratio of gas flow (Oxygen /Argon)***

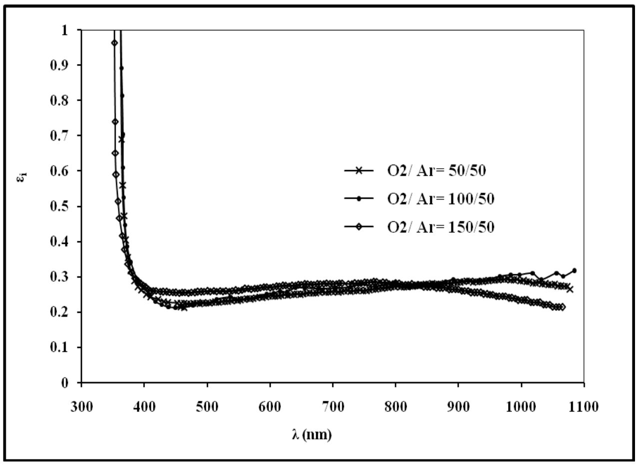


***Fig. 8: Imaginary part of dielectric constant ($\varepsilon_r$) of $TiO_2$ films vs. wavelength formed at various ratio of gas flow (Oxygen/Argon)***

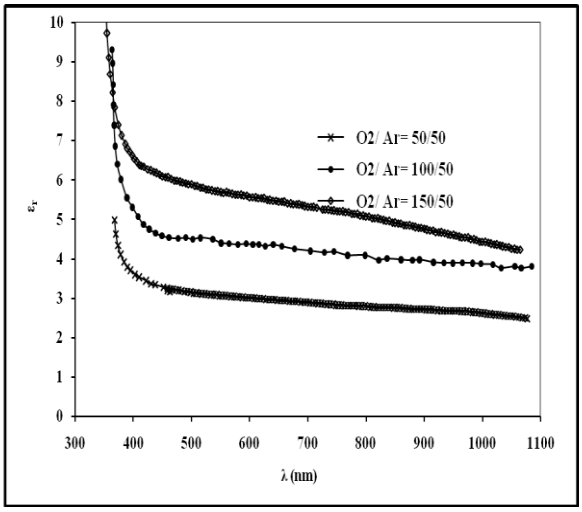


***Fig. 9: Real part of dielectric constant ($\varepsilon_i$) of $TiO_2$ films vs. wavelength formed at various ratio of gas flow (Oxygen/Argon)***

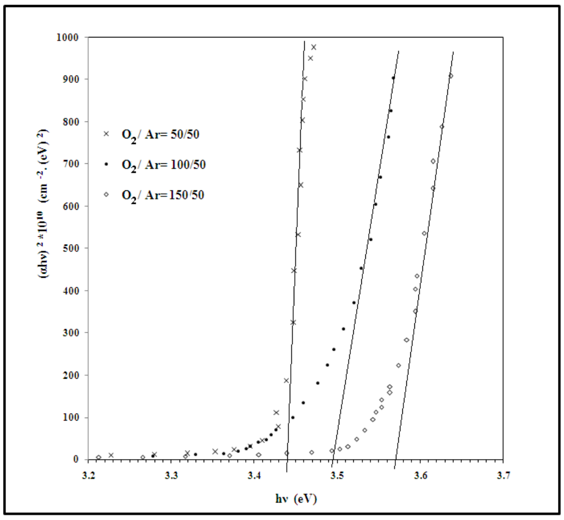


***Fig. 10: $(\alpha h\upsilon)^2$ versus energy curves of $TiO_2$ films vs. wavelength formed at various ratio of gas flow (Oxygen /Argon)***

**Conclusions**

Titanium oxide films were deposited by DC magnetron sputtering using different $O_2$/Ar gas flow ratios. XRD results show that rutile, anatase and brookite phases. The grains size increases with increasing of oxygen flow rate and the thin film become more transmittance. The energygap increases when the ratio of oxygen increases.

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