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# OPTICAL INVESTIGATIONS OF $Nb_2O_5$ AT DIFFERENT TEMPERATURES FOR OPTOELECTRONIC DEVICES

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Effect of different substrate temperatures on the optical properties and some of the optical constants of $Nb_2O_5$ thin films is conducted in this work. Estimated optical band gap and optical constant confirms the dependency of $Nb_2O_5$ thin films on the substrate temperatures. The band gap in the range of 2.8 to 3.5 eV is directly related to the solution properties. The energy gap at optimum preparation state ensures the development of semiconducting material that suits solar cell and other optoelectronics application.

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*Keywords:* Treatment temperature, Optical Properties, Optical constant, $Nb_2O_5$ films

## 1. Introduction

The $Nb_2O_5$ thin films Interest could be dated back to the early fortieth from the last century, when the first polymorphs niobium oxide has been studied [1-3]. Niobium pentoxide, in the recent years has emerged as a several purpose material that attracts the attention and a wide scientific interest. It is one of the popular transparent oxides semiconductor materials [3-6]. This material is a transparent in the Uv region because of its wide band gap, water-insoluble and air-stable material. It has a relatively complex structure that displays a polymorphous structure depended on preparation method and condition [7, 8]. These polymorphic structures give rise to an important series of phases. All of them based on ($NbO_6$) octahedral groups, forming different arrangement from the rectangular columns or blocks [9, 10]. It is abundant material in nature, thermodynamically stable, with high corrosion resistance [11-13].

$Nb_2O_5$ thin films are widely used in several now day application such as optoelectronic devices, optical coatings, catalysis, gas sensors, photocell, Ec devices and others due to their interesting properties, such as wide band gap, elevated index of refraction, very good thermal chemical and stability [14-21]. Attention on $Nb_2O_5$, has obtained more momentum due to their applications, especially, nanostructured $Nb_2O_5$ in solar cells, batteries, photo-detectors and other electronic devices [22-25].

Previous study on the electrical properties of this material reveals the dependent of its energy gap on preparation condition, wide energy gap range was obtained extended from (2.1-3.6). in oure previous study, we investigate the effect of ultrasound vibration on the optical properties [26] , on other work effect of ammonium molarity concentration was done, it reveals a dramatic change in optical properties with molar ratio, [27].

In this work, the effect of substrate temperatures on the optical properties and some optical constants of $Nb_2O_5$ thin films were examined and analyzed. This work also reveals cost-effective and simple deposition method that has been used to deposit $Nb_2O_5$ thin films on quartz substrate.

## 2. Experimental work

By using ultra-purity (99.99%) of niobium pentoxide powder (0.2 g), the required $Nb_2O_5$ colloidal solution was obtained by solving the powder in hydrofluoric acid (HF) in water path at

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100 °C and continuous stirring for 1 hour as until the solution became totally transparence giving indication for totally salvation for $Nb_2O_5$ powder according to equation (2-1), then DIW and ethanol were added to dilute the solution, Heat treatment to the substrate was done using burn furnace () in static air for 1 hour using different treatment temperature (200, 300, 400,500,600, 700) °C with (10°C/min) heating rate. Then the samples cooled down over night to room temperature [28].

The thin films were prepared using layer by layer spin coating growth (HOLMARC HO-TH-05) using (1500 rpm) speed for 1 min duration then the film was dried in drying oven with 100°C for (15 min). This process repeated three times producing three layer of films. The optical results was investigated using (T60) UV-Vis spectrophotometer is used to measure the transmittance of $Nb_2O_5$ thin films deposited on quartz substrate in the range (200-900) nm. For every scan the background correction is possessed. The transmittance data can be utilized to calculate absorption coefficient, the optical energy band gap ($E_g$) of the films using the following equations [29-33]:

$$(\alpha h\nu) = B(h\nu - Eg)^{1/2} \quad (1)$$

where B is a constant and α is the absorption coefficient its value depended on the thickness (t) and the transmitting ($T_{rans}$)

$$\alpha = \frac{1}{t} \ln \frac{1}{T_{rans}} \quad (2)$$

where λ′ the incident photon wavelength, t is the thickness of the film [34, 35].

Urbach energy (*Eu*) was also calculated by measure the slope of the straight line fitted the linear part of the curve plotted between lnα vs. photon energy relying on the following formula [36, 37]:

$$\alpha_{h\upsilon} = \alpha_0 \exp \frac{h\upsilon}{E_u} \quad (3)$$

## 3. Results and discussion

Optical properties of the prepared $Nb_2O_5$ thin films were investigated. Fig. 1 shows the transmission spectrum of the prepared films treated at different temperature ranged from (200-700)°C.

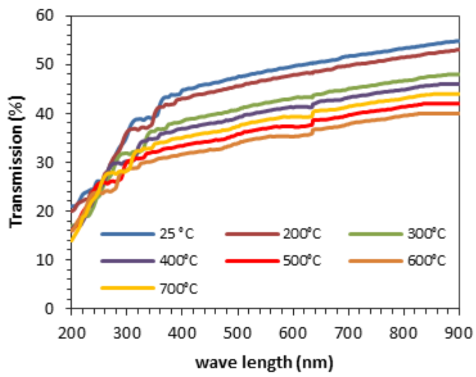


*Fig. 1. Transmission spectrum of $Nb_2O_5$ the thin films prepared at 12 mol/L molarity treated at different heat treatment temperatures.*

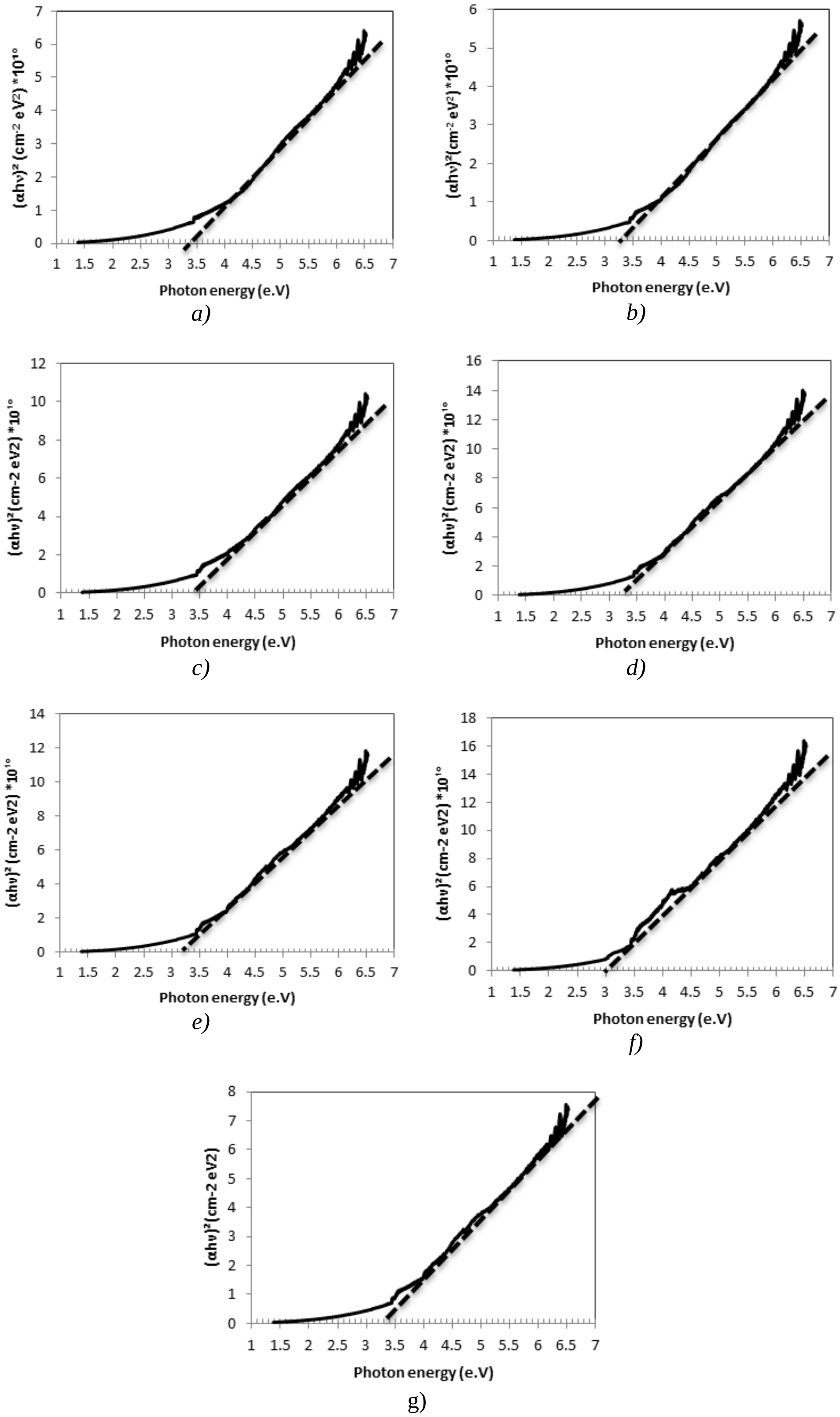


*Fig. 2. Energy gap of $Nb_2O_5$ thin films prepared in 12 mol/L molarity and treated in different heat treatment temperatures*
*a): without, b):200°C, c):300°C, d):400°C, e):500°C, f):600°C, g)G:700°C.*

The transmission spectrum of the thin films was decreased as the temperature increased reaching its minimum value at 600 °C, this may impute to the presence of oxygen vacancies. The formation of defects of oxygen increases the concentration of the localized states in the band structure [38]. It's also attributed to scattering from grain boundaries due to the increasing in the grain size with increasing in the annealing temperature. The increasing in the grain size also contributed on the decreasing of the transmission by increasing the absorption associated with the reduction of the mechanical stress as a result to the lattice distortion in the grain boundary regions which influence the electronic structure and, hence, the below-band-edge optical absorption [39]. Farther increasing in treating temperature caused an increasing in the transmission.

Relying on the transmission spectrum the energy gap of the prepared films were extracted using equation (1), relation between $(\alpha h\nu)^2$ and photon energy for $Nb_2O_5$ thin film treated at different heat treatment temperatures were shown in Fig. 2, and its value was displayed in Fig. 3.

According to Fig. 3 a very close energy gap value could be recognize, with a relative variation with temperature. The band gap starts to decreases slightly when the temperature increased hence the re-crystallization begins.

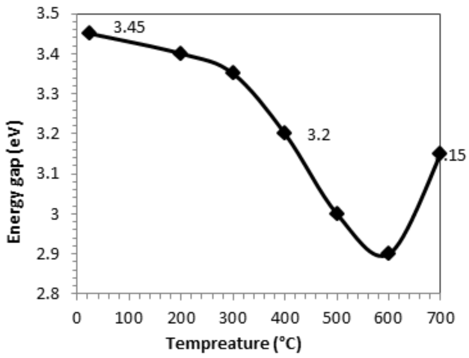


*Fig. 3. Energy gap value as a function to heat treatment temperature for $Nb_2O_5$ thin films prepared in 12 mol/L molarity.*

The reduced energy gap value related to the presence of the unsaturated bonds that caused the formation of the localized tail states in the energy gap as shown in Fig. 4. The high concentration presence of these states is accountable on the reduction of bandgap for films treated at different temperatures. An increase in the average grain size was combined with this transformation; as a results, a drastic effect of crystalline phases on optical gap can by explained, due to the increase in the surface dangling bonds around the crystallites during the crystallization process. In addition, an increase in the annealing temperature to 700 °C results in breaking up the film crystallites into smaller one, which resulting in increase the number dangling bonds at the surface, so that some types of defects would be formed. These defects lead to the decrease of the optical gap, similar results could be found elsewhere [40].

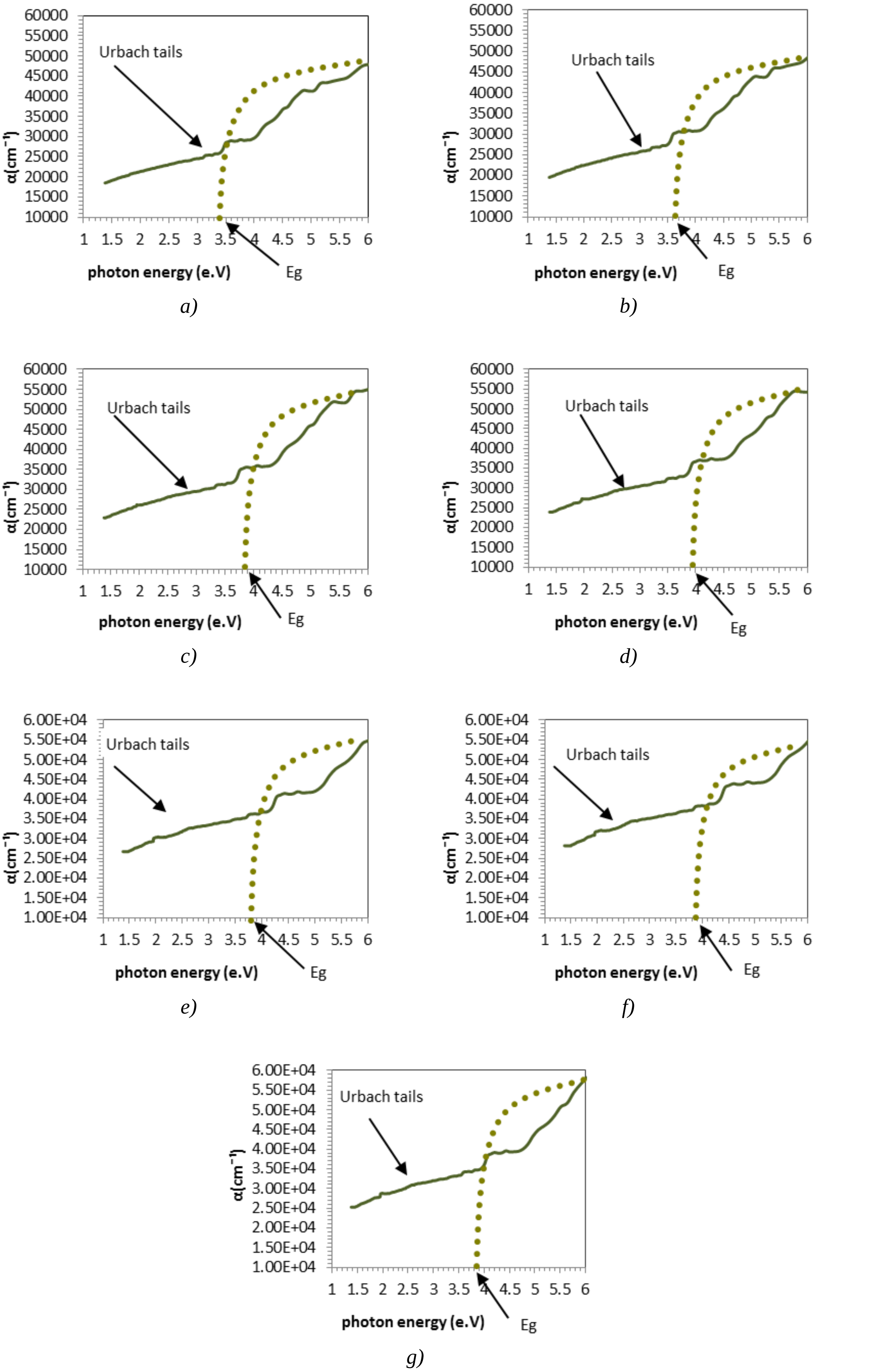


*Fig. 4. The relation between the absorption coefficient and the absorbed photon energy showing the absorption tails for $Nb_2O_5$ thin films prepared at 12 mol/L molarity and treated in different heat treatment temperatures a): without, b):200°C, c):300°C, d):400°C, e):500°C, f):600°C, g):700°C.*

## 4. Conclusions

$Nb_2O_5$ was successfully deposited at optimum different substrate temperatures, and 12 Mol/l. The Niobium pentoxide colloidal suspension was deposited using a simple and easy technique with the vastly available raw material. The optical properties and some of the optical constants of the prepared $Nb_2O_5$ thin films confirmed the high affectivity of the added ammonium concentration on these characteristics. An unusual behavior in the energy gap, the optical properties indicated increment in the absorbance and decrement in the band gap as the temperatures increased to 600 $^oC$. Some of estimated optical constants at the optimum condition verify the films suitability for renewable energy application.

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