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Investigation of Structural and Optical properties of Tantalum Oxide Nano layers Deposited by Electron Gun Evaporation Method as Function of Thickness and Vertical Deposition Angle

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Abstract

Tantalum oxide Nano layers were deposition on glass substrates with four different thicknesses 30, 60, 90 and 120 degrees in vertical deposition angle, under HV condition at room temperature with electron gun by physical evaporation deposition method. Other deposition conditions were the same for all layers. Their topography, roughness, crystallography, surface morphology and element analysis were investigated by AFM, X- ray diffraction, FESEM and EDAX analysis. Optical reflectance measured in the UV-VIS wavelength range by spectrophotometer. By using Kramers-Kronig relations on reflectivity curves other optical parameters such as, real and imaginary part of reflective index, real and imaginary part of dielectric constant, absorption coefficient and optical band gap energy were calculated.

Keywords: Tantalum oxide; Thin film; Structure; Optical properties

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Introduction

Optical thin films and optical devices have attracted much attention from both academic research and engineering application, due to the rapid development of opto-electrics and semiconductor techniques in recent decades [1–3]. Each layer plays important roles in the functionally optical properties. Optical constants, such as refractive indices and extinction coefficient as well as optical thickness of the thin films, are very important parameters in optical design and device fabrication [4,5]. Because of good chemical and thermal stability, high refractive index, high transmission and low extinction coefficient in visible spectrum, Ta_2O_5 thin films are used in optical applications, such as anti-reflecting coatings, optical waveguides, interference coatings and photoelectric conversion [6,7].

Some of these applications include resistive switching memory, anti-reflective (AR) coatings (solar cells, for example), optical waveguides, and electroluminescent devices, and used as insulators in the storage capacitors of dynamic storage devices [8-10].

Methods and conditions of deposition affect optical and structural properties of Ta_2O_5 thin films. Various techniques have been used to deposit Ta_2O_5 thin films, such as chemical vapor deposition, electron beam evaporation, thermal oxidation, ion beam sputtering, RF sputtering and atomic layer deposition (ALD) [11-16].

By studying the reflectance spectra of layers deposited on solid surfaces optical constants for layers (real and imaginary part of refractive index n and k) can be determined [17]. There are many different methods for determining the optical constants of materials. One of the most common techniques that have been used to determine the optical constants over the whole measurement range is Kramers-Kronig analysis [18]. In this study, production of tantalum oxide nano layers were deposition on glass substrates, in under HV condition at room temperature by electron gun evaporation method and investigation about their structural and optical properties as a function of with different thicknesses in vertical deposition angle and other deposition conditions were the same for all layers.

The objective of this research includes detailed Nano structural characterization of the coated layers. The layers have been characterized by different techniques such as X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM), Energy dispersive X-ray spectroscopy (EDAX), Atomic force microscopy (AFM) and optical spectra's by Spectrophotometry and optical properties by Kramers-Kronig relations.

Materials and Methods

Tantalum oxide nano layers were prepared on glass substrates $(1 \times 20 \times 20)\ mm^3$ using an ETS160 system with a pressure of 3×10^{-7} torr. The layers were obtained in condition of high vacum, with using electron gun by physical evaporation deposition method (PVD) (Edwards E19A3). The deposition rate used by us was 0.2 A°/S the purity of tantalum oxide was 99/9%. The temperature of the substrates was kept constant (300 K). Before deposition process substrates were cleaned in heated deionized water (within 15 min) then acetone (within 15 min) and ethanol (within 15 min) by ultrasonic. The thickness of the layers were 30, 60, 90 and 120 nm the obtained by quartz crystal technique (Sigma Instrument, SQM-160, USA) deposition angle of the layers were vertical degree. Standard 2 mm thick glass slides were used as substrates.

For the study of the crystalline, morphological evolution of the coting we used XRD (STADI MP, STOE, Germany) and FESEM (S-1400, Hitachi, Japan), respectively. While the surface physical morphology and roughness were obtained by means of AFM (Nt-mdt scanning probe microscope BLOO, Russia, with low stress silicon nitride tip of less than 200 A radius and tip opening of 18) analysis. The transmittance spectra, were measured by using a UV-VIS spectrophotometer (stellar, American) in the wavelength range from 400-850 nm. The optical constant of our samples were derived on the basis of standard Kramers-Kronig relations using computer techniques.

Results and Discussion

Structural properties of Ta_2O_5 nano layers

X-Ray Diffraction analysis: **Figure 1** shows X-ray diffraction images of four layers of tantalum oxide made at vertical deposition angle on glass substrate and in four different thicknesses. As can be seen, all layers are formed as amorphous and no specific style can be seen in a- b- c- d of **Figure 1**.

Energy dispersive X-ray spectroscopy: EDAX results are shown in figure for the layers produced in this work **(Figure 2).** Shows the EDAX diagrams related of tantalum oxide made at vertical deposition angle on glass substrate and in four different thicknesses. As we can see, by increasing the thickness from 30 to 120 nm the amount of tantalum atoms has had an increasing that was predictable and other elements related to the substrate ingredients are almost constant **(Figures 3-5).**

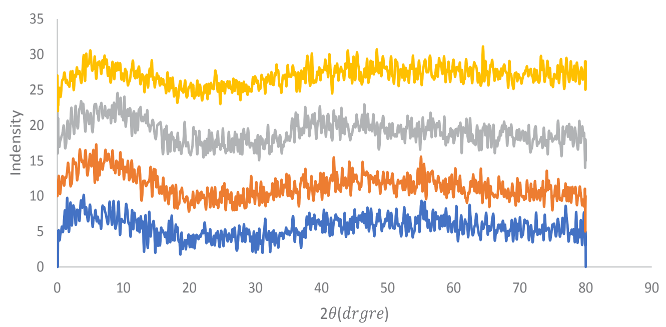

Figure 1 X-ray diffraction images (XRD), of tantalum oxide Nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm

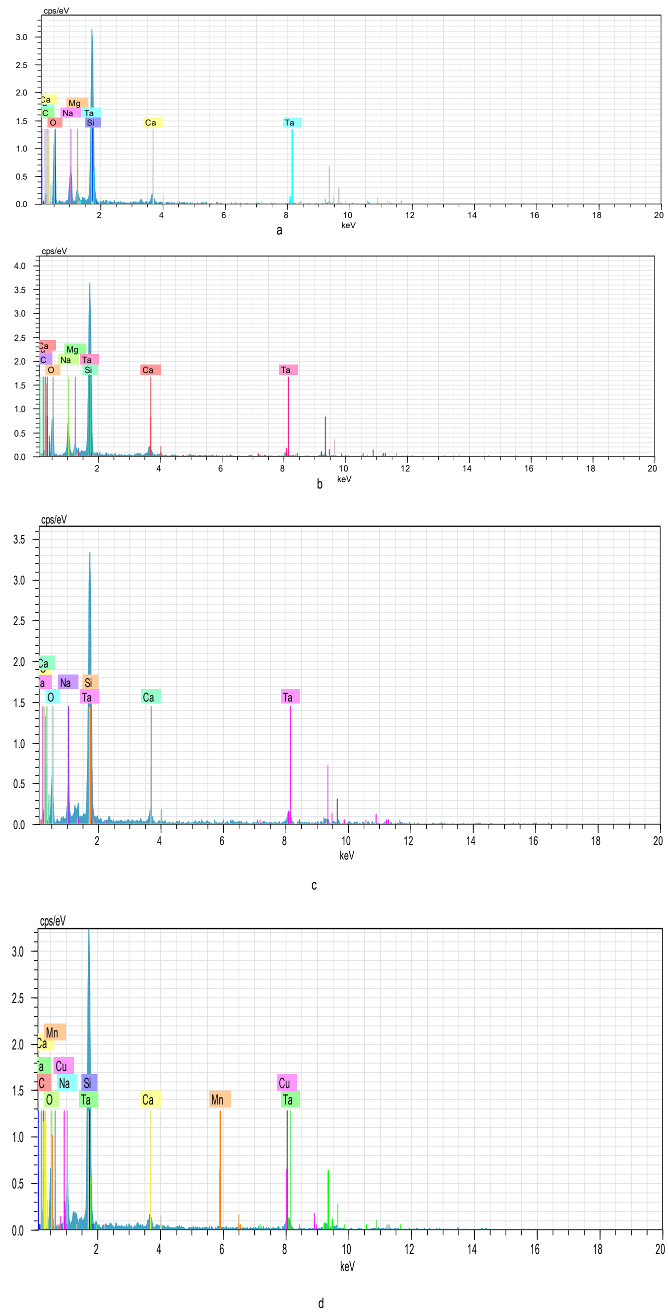

Figure 2 Energy dispersive X-ray spectroscopy images (EDAX), of tantalum oxide Nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

Field emission Scanning Electron Microscopy analysis

The nanostructures Ta_2O_5 of layers were investigated by using scanning electron microscopy. **Figure 6** shows field emission scanning electron microscopy images (FESEM) related to tantalum oxide samples on glass substrate at vertical deposition angle and different thicknesses made by electron gun. The nucleation level is observed on the surface. By increasing the thickness to 60 nm, growth and accession and integration has been observed which is visible as interconnected islands. In **Figure 3** the accession and integration is complete and the surface is full of tantalum oxide grains. (90 nm) and by increasing the thickness to 120 nm in **Figure 3** re-nucleation is formed on the layer **(Figure 3).**

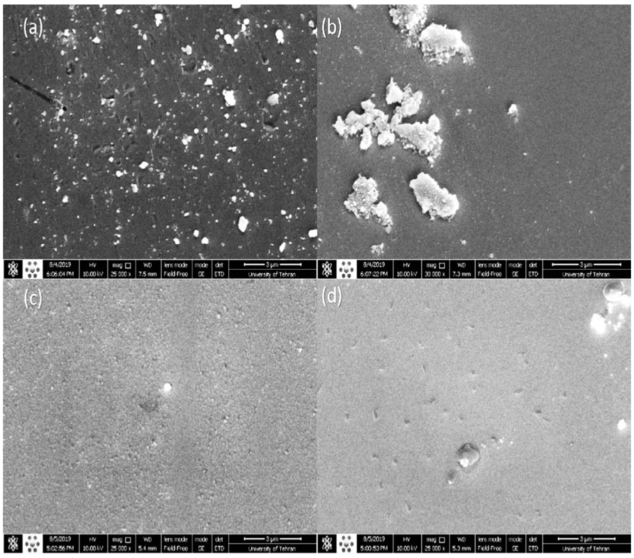

Figure 3 Field emission scanning electron microscopy images (FESEM), of tantalum oxide Nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm

Atomic force microscopy analysis

Figure 4 shows two-dimensional images of atomic force microscopy for tantalum oxide Nano layers Ta_2O_5 on the glass substrate at a vertical deposition angle made by an electron gun related to this research. As can be seen from figure, in the thickness of 30 nm, tantalum oxide grains are aggregated in some places and the rest of the substrate is empty. By increasing the thickness to 60 nm in figure, the surface is homogeneously filled with two-dimensional tiny grains and circular tantalum oxide shapes with empty spaces between them. In figure, the surface of the glass substrate is filled with four bladed grains (in the form of dentin) was observed in two dimension and the empty spaces of the substrate were reduced. In figure, the surface filled with tiny and big grains is formed circularly on the substrate and we see a relatively smooth structure in two dimension. Empty spaces have dropped dramatically. Through the calculations of J micro-Vision software, the size of the calculated grain for the four vertical deposition samples was observed as the **(Table 1).** As could be seen from thicknesses of 60 nm and 90 nm, the size of the formed grains is fixed on the surface. In 120 nm thickness, due to the insertion and integration due to the growth of grain size, the size of the grains is larger. However, at 30 nm, the deposition

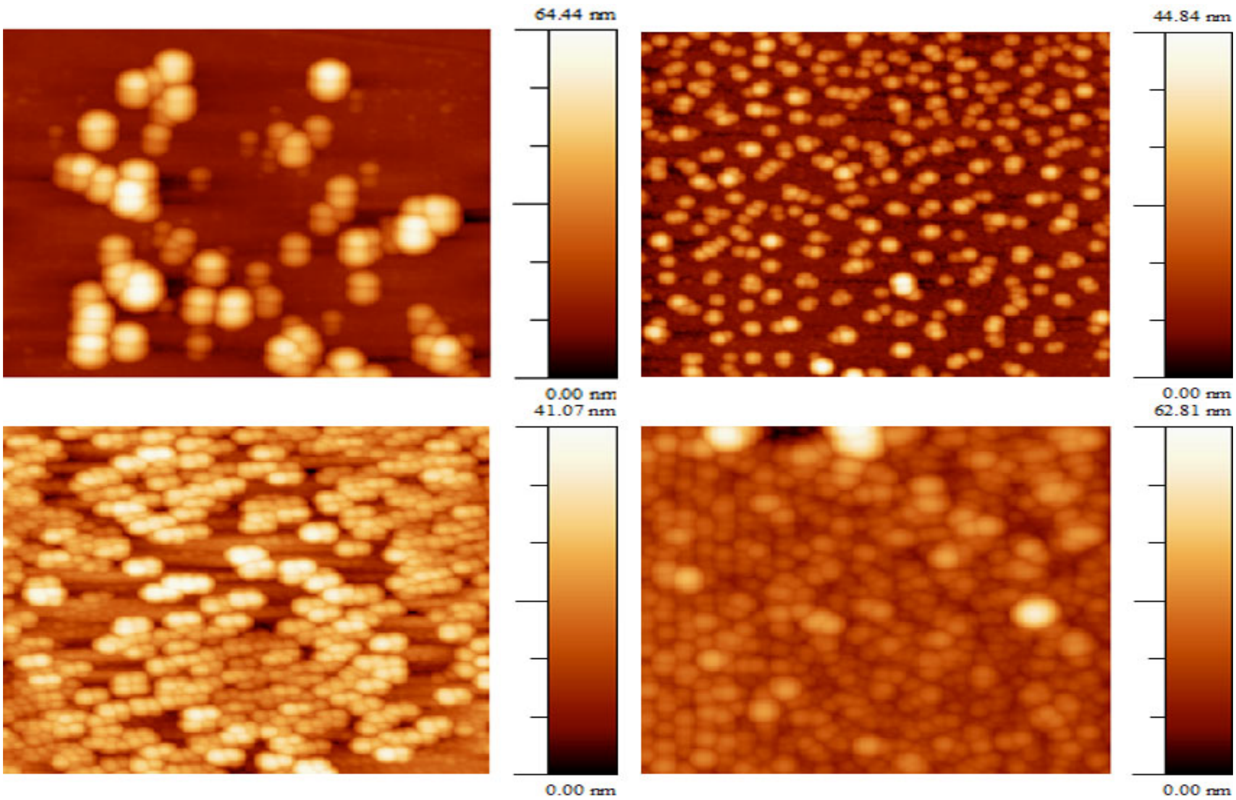

Figure 4 Two-dimensional images of atomic force microscopy (AFM), of tantalum oxide nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

rate was probably slightly lower and the measurement error of the device increased the grain size **(Figure 4).** In figure Gaussian diagrams related to the above diagrams indicate the distribution of Gaussian functions of the grains on the surface **(Figure 5).** In figure the diagram 2 shows the hardness values of the surface for the above four samples **(Figure 6).** As can be seen, by increasing the thickness of the layer, the hardness of the surface is reduced and the layer is formed as homogenization. Figure shows atomic force microscopic images in dimensions of (5 μm × 5 μm) for tantalum oxide samples made on the glass substrate at vertical deposition angle using electron gun method. Figure shows 3D image of atomic force microscope with a thickness of 30 nm. As can be seen, the surface is formed in some places as conical beads of domed tip and back together. The empty spaces on the substrate are strikingly visible. In figure thickness is increased to 60 nm and the surface is filled with needle-shaped beads with empty spaces. This volumetric fraction of holes has been reduced. In figure by increasing the thickness to 120 nm, the surface is homogeneous and in some places domed grains are seen that the volume of holes has decrease **(Figure 7).**

Table 1 The size of grains of nano layer (Ta_2O_5/glass) of vertical deposition angle.

Thickness nm)	Grain size (μm)
30	0.09
60	0.07
90	0.07
120	0.09

Optical properties and Kramers-Kronig relations

In this work Kramers-Kronig relations were used to calculate the phase angle $\theta(E)$ that we have explained in our earlier works [17,18], extensively.

$$\theta(E) = -\frac{E}{\pi}\int_0^{E_2}\frac{\mathrm{h}\;R(E)-\mathrm{h}\;R(E_0)}{E^2-E_0^2}dE + \frac{1}{2\pi}\ln[\frac{R(E)}{R(E_2)}]\mathrm{h}\;\frac{E_2+E}{|E_2-E|}+\frac{1}{\pi}\sum_{n=0}^{\infty}[4(\frac{E}{E_2})^{2n+1}](2n+1) \quad (1)$$

Where E denotes the photon energy, E_2 the asymptotic limitation of the free-electron energy, and R(E) the reflectance. Hence, the θ(E) can be calculated. Then the real and imaginary parts of the refractive index were calculated, from which other parameters were obtained.

The results of optical properties are as follows:

The diagrams of the real part show the refractive index of tantalum oxide Nano layers on the glass substrate at vertical deposition angle with different thicknesses **(Figure 8).** As we can see, with increasing thickness, the increased absorption zones are observed in figure peak at energy of 3.1 eV. By increasing the thickness to 60 nm, the energy shift is created and our peak is observed at 3.8 eV. By increasing the thickness to 90 nm, two peaks appeared at the energy of 2 and 3.3 eV. By increasing the thickness to 120 nm in, our two peaks, the energy shift has been observed as 2.2 and 3.55 eV **(Figure 8).**

The extinction coefficient diagrams of tantalum oxide samples are visible on the glass substrate at vertical deposition angle and different thicknesses **(Figure 9).** In general, the extinction

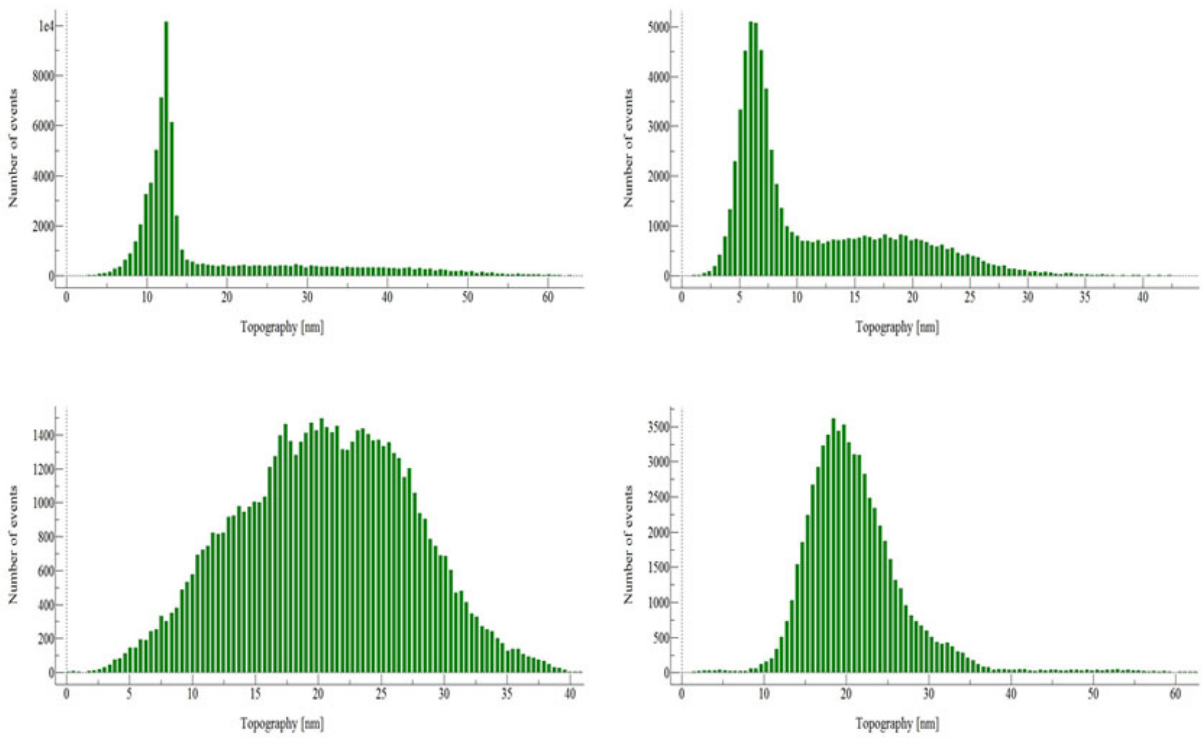

Figure 5 Diagrams to topographic, of tantalum oxide nano layers on glass substrate (Ta_2O_5 /glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

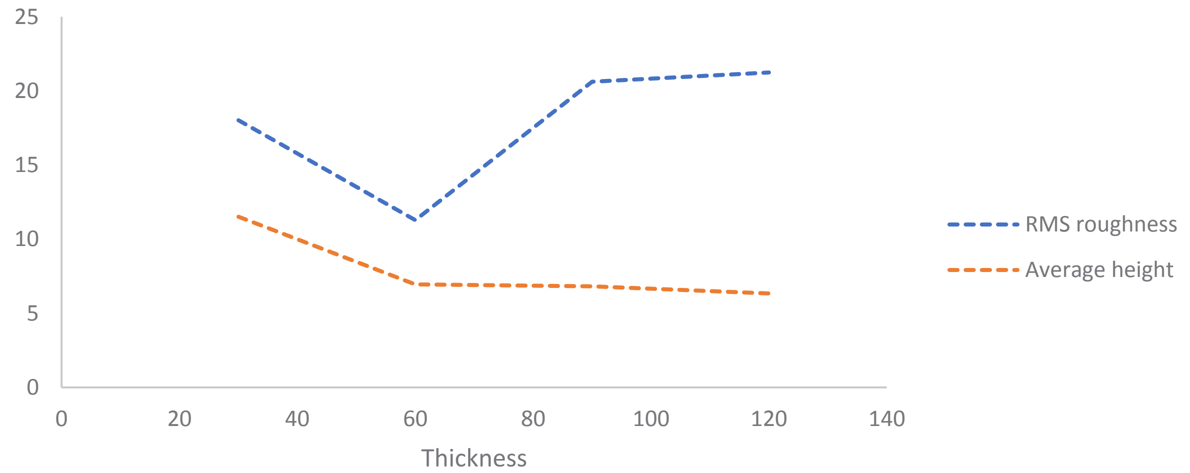

Figure 6 Diagram the hardness values of tantalum oxide nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method.

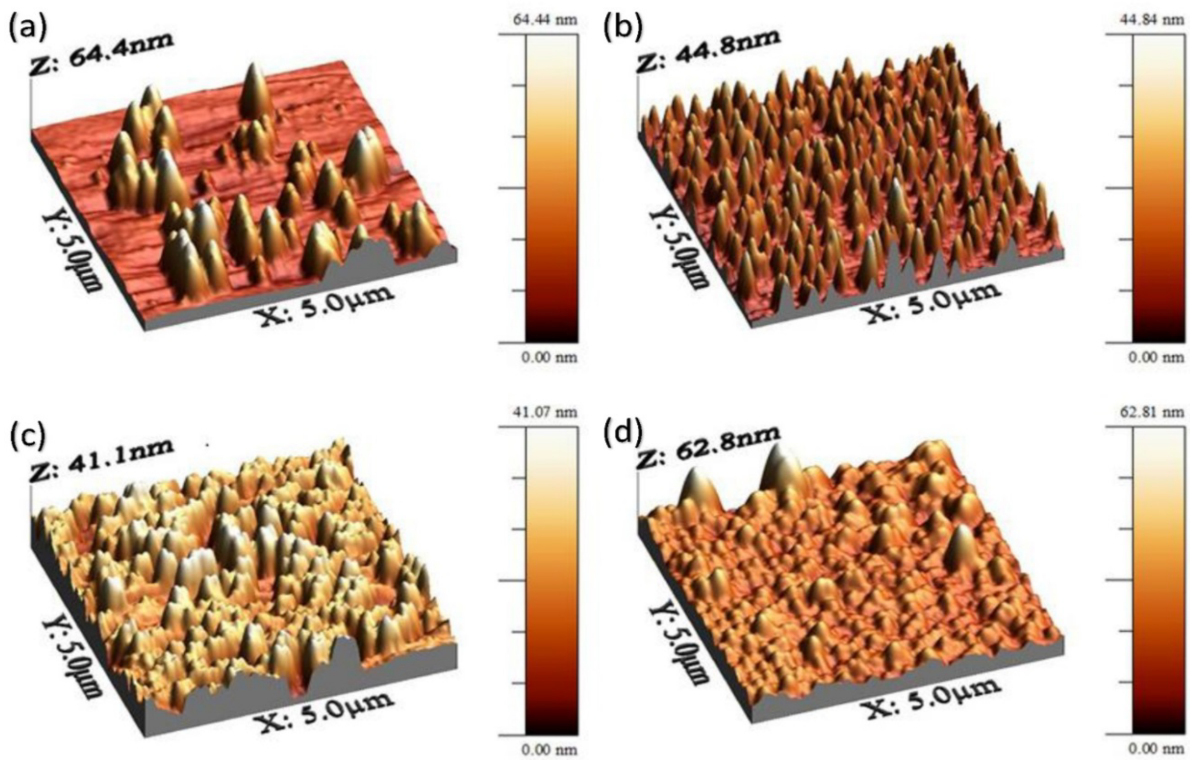

Figure 7 Three-dimensional images of atomic force microscopy (AFM), of tantalum oxide nano layers on glass substrate (Ta_2O_5/glass) made at vertical deposition angle by electron gun method (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

coefficient has increased with increasing thickness. This means that absorption increases and the absorption edges of the absorption zones are visible in the real part.

Diagrams in figure show the real part of the dielectric function of tantalum oxide Nano layers on the glass substrate at vertical deposition angle and in different thicknesses **(Figure 10).**

By increasing the thickness of these layers dielectric properties have been increased. The observed peaks in 3 to 3.5 eV are evident in all diagrams.

Diagrams of the imaginary part of the dielectric function are plotted in **Figure 11**. As can be seen, with increasing thickness, absorption in the layers has generally also increased.

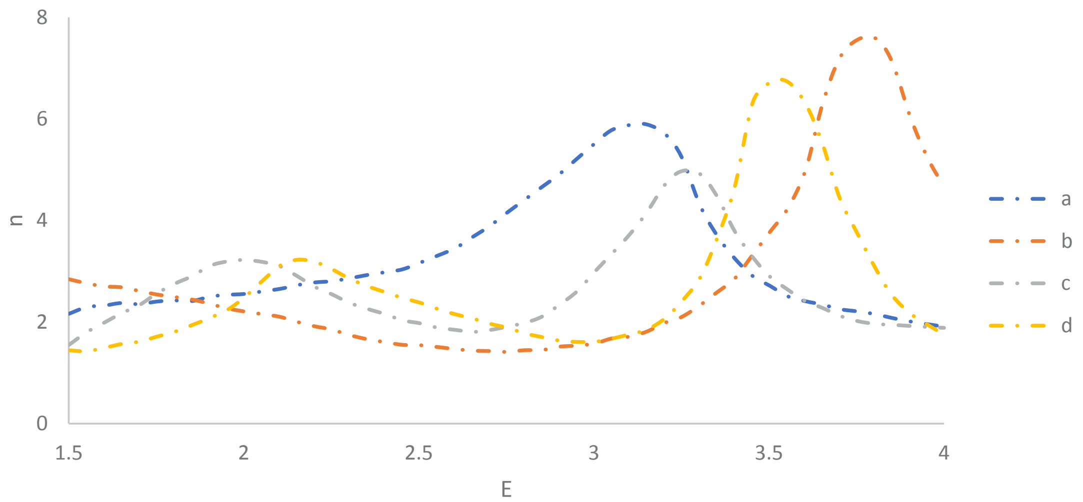

Figure 8 Comparison of prognostic related genes expression in 7 NSCLC patients in lung cancer tissues and paracancerous tissues.

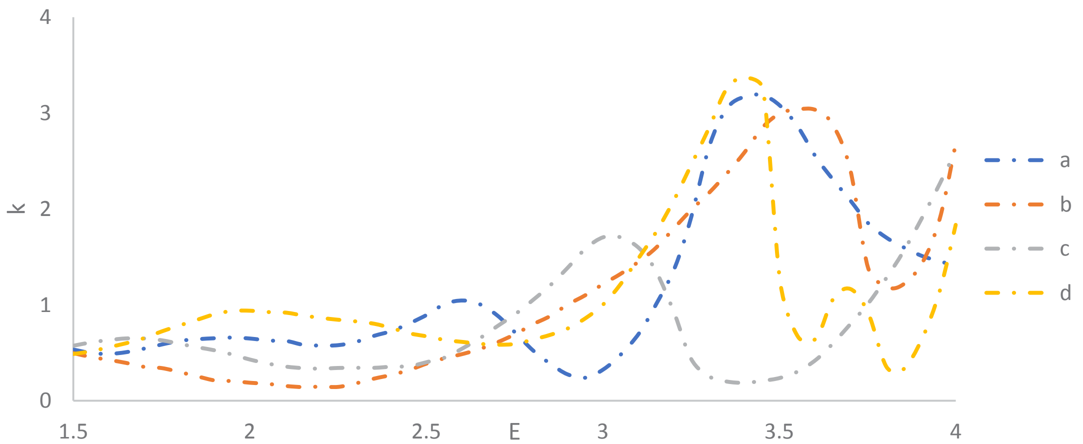

Figure 9 Comparison of prognostic related genes expression in 7 NSCLC patients in lung cancer tissues and paracancerous tissues.

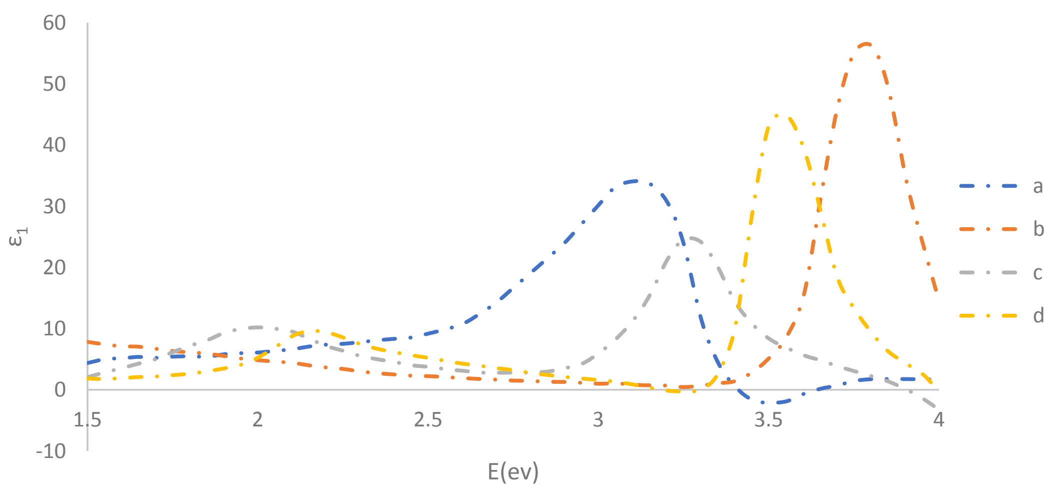

Figure 10 Diagrams of the real part of the dielectric function of nano-tantalum oxide layers on the glass substrate at a vertical deposition angle made by electron gun (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

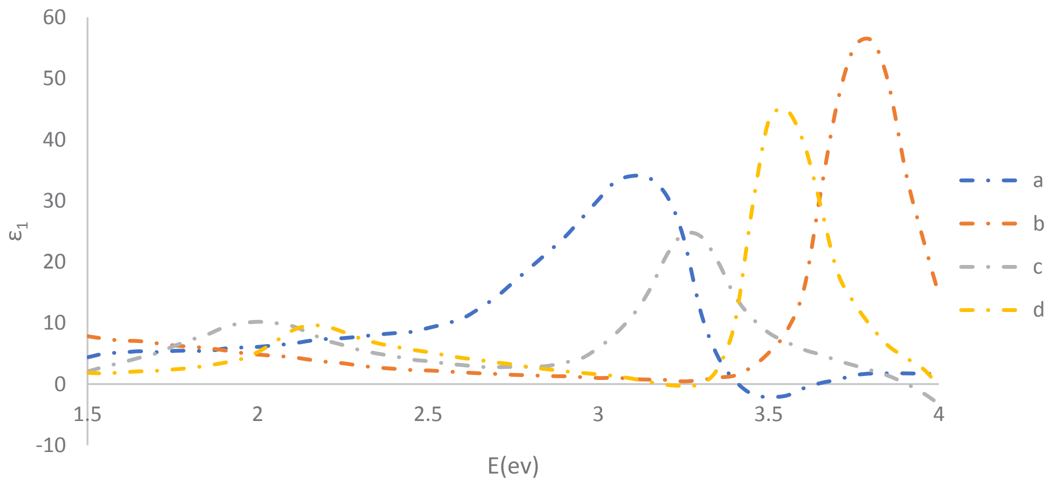

Figure 10 Diagrams of the real part of the dielectric function of nano-tantalum oxide layers on the glass substrate at a vertical deposition angle made by electron gun (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

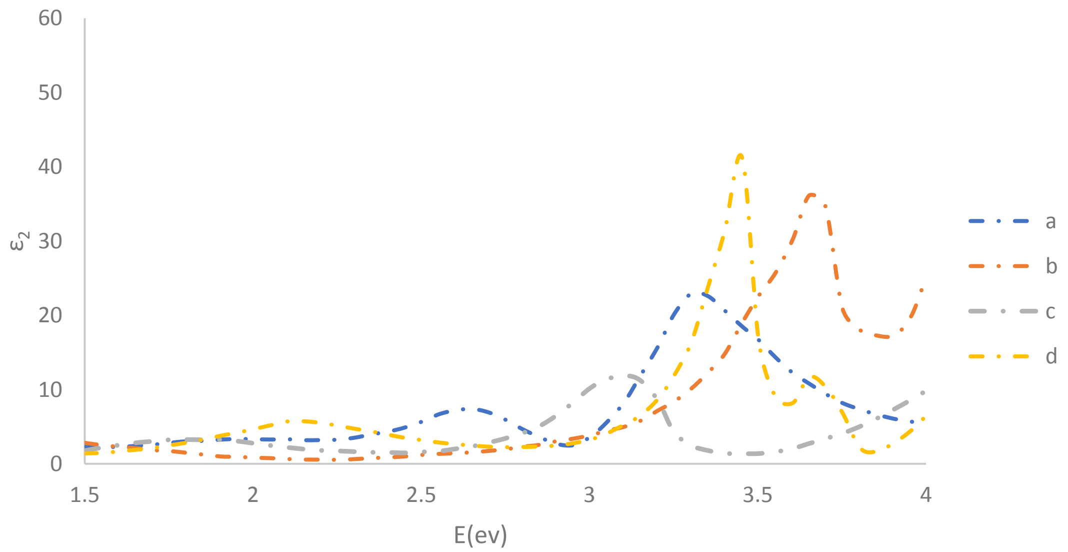

Figure 11 Diagrams of the imaginary part of the dielectric function of nano-tantalum oxide layers on the glass substrate at a vertical deposition angle made by electron gun (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

Figures show the absorption coefficients and optical band gap related to tantalum oxide Nano layers on the glass substrate made by electron gun at vertical deposition angle and different thicknesses **(Figures 12 and 13).**

According to figure, it can be seen with increasing thickness, absorption coefficient and absorption peaks has increased, resulting a decrease in the volume fraction of holes in the built-in samples **(Figure 12).**

In figure, the optical band gap of the above samples has been calculated. As can be seen, with increasing thickness, band gap has also increased and dielectric properties of the layers have also increased **(Figure 13).** Table shows the energy band gap values of the above samples **(Table 2).**

Chalcopyrite structure Ta_2O_5 has a direct band gap, so that the optical band gap (E_g) of the layers can be calculated with the following relationship [19]:

$$(\alpha h\nu)^2 = (h\nu - E_g), \qquad (2)$$

Where hv is photon energy and experimental absorption coefficient is given as:

$$\alpha = \frac{2E}{\hbar c} k(E) \qquad (3)$$

Where c is the velocity of light and k(E) is the imaginary part of refractive index. We depict the band gap energy for layers produced in this work in **Figure 13**. **Table 2** shows the values of band energy for the layers produced in this work.

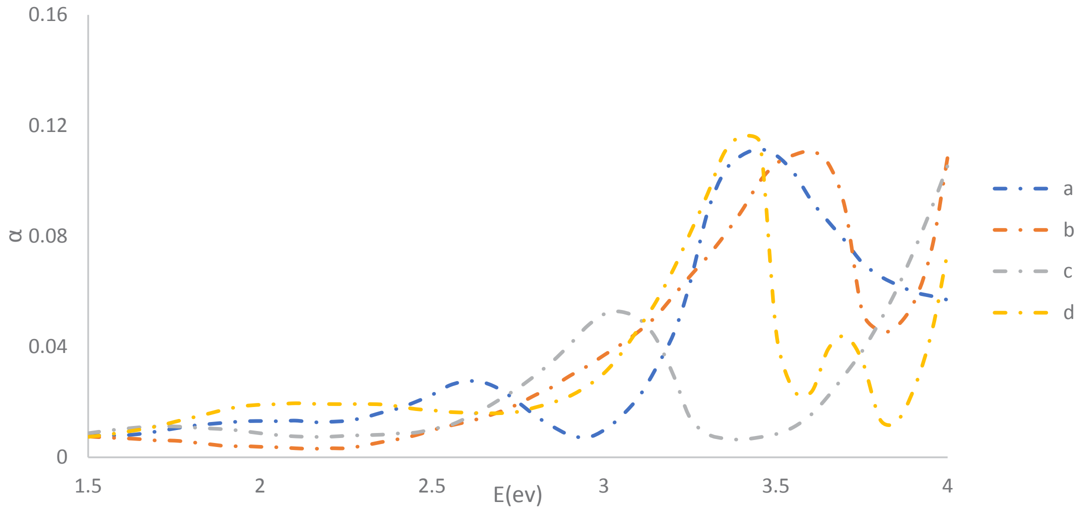

Figure 12 Diagrams of absorption coefficient of tantalum oxide nano layers on glass substrate at vertical deposition angle made by electron gun (a) 30 nm, (b) 60 nm, (c) 90 nm and (d) 120 nm.

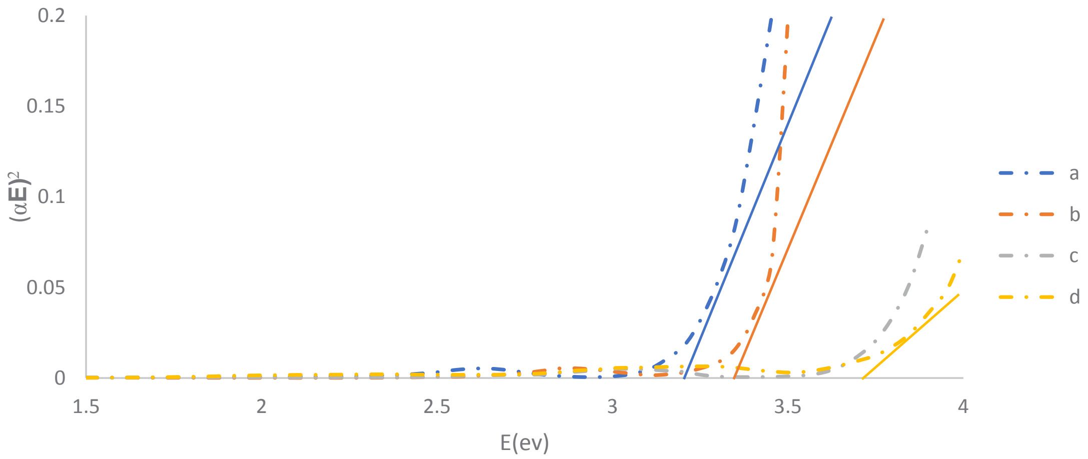

Figure 13 Diagrams of energy band gap of tantalum oxide nano layers on glass substrate at vertical deposition angle made by electron gun (a) 30 nm, (b) 60 nm, (c) 90nm and (d) 120 nm.

Table 2 Band gap energy values of nano layer (Ta_2O_5/glass) of vertical deposition angle.

Thickness (nm)	Band gap (eV)
30	3.1
60	3.3
90	3.6
120	3.7

Conclusion

In this study, we investigated the structural and optical properties of tantalum oxide Nano layers Ta_2O_5 on the glass substrate with vertical deposition angle in four thicknesses of 30, 60, 90 and 120 nm made by the corresponding electron gun. In atomic force microscopy analysis, the thicknesses of 60 nm and 90 nm of grain size formed on the surface are constant and by increasing the thickness to 120 nm due to the accession and integration due to growth, the grain size is larger. Surface roughness is reduced by increasing the thickness of the layer and the layer is shaped as homogenization. In field emission scanning electron microscopy images (FESEM) related to tantalum oxide samples on glass substrate at vertical deposition angle and different thicknesses made by electron gun. Nucleation, growth and accession and integration observed as interconnected islands, complete accession and reintegration and re-nucleation were observed for thicknesses of 30, 60, 90 and 120 nm, respectively. There was no specific peak in x-ray diffraction images due to amorphous layers. In investigating the optical properties, we concluded that in the optical coefficients: in the real part, the refractive index of tantalum oxide by increasing the thickness, the energy shift has been created. In general, the extinction coefficient has increased with increasing thickness. That is, absorption increases. The dielectric properties of the layers have also increased with increasing thickness and absorption has generally increased with increasing the thickness of absorption coefficient and increased absorption peaks, which indicates a decrease in the volume fraction of holes in the made samples. By increasing the thickness, the band gap has also increased and the dielectric properties of the layers have also increased.

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