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Influencing of Substrates Types on the Optical Properties of Nickel Oxide Films Deposited by Silar Method

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Abstract

In this study, some optical properties of nickel oxide (NiO) films deposited on different glass substrates (ITO, FTO, glass) were characterized by the successive ionic layer adsorption and reaction (SILAR) method. All films were determined to form in the cubic phase of NiO according to the Joint Committee on Powder Diffraction Standards (JCPDS:01-073-1519) card. Some optical properties such as the energy gap were measured as the values of the direct optical Energy gap changed in the range (3.81-3.88 eV). The results showed that the transmittance values in the visible range of the samples gradually increased with wavelength (from 15% to 54%), with a clear superiority in the transmittance values of the films deposited on ITO substrates. Similar to the transmittance and absorbance values of the samples, the films deposited on (glass) showed linear behavior, in contrast to the rest of the samples deposited on FTO and ITO substrates, which showed exponential behavior with higher transmittance. Similar light absorption behavior was observed across all samples, with a proportional decrease in absorption values with increasing wavelength. The films had identical results to previous studies, indicating the reliability of the SILAR method in film preparation and characterization. The maximum absorption peaks are limited to the short wavelength range (300-350 nm).

Introduction

Thin films have different properties than in the bulk state, due to the interaction of the films with the substrates deposited on them [1]. Accordingly, the reaction processes during deposition on different substrates are one of the means of obtaining different results that can be characterized and the possibility of their application determined. Although determining the relationship between deposition parameters and morphology of deposited thin films is very complex due to the interaction of many factors affecting the nucleation and growth stages, it is still possible to find some common stereotypes for a variety of thin films that define the method, which Through which the adsorbed atoms are incorporated into the final growth process of thin films when the atoms collide with the substrates [2].

Previous studies paved the way for the selection of fluorine-doped tin oxide (FTO), which exhibits similar transmittance to ITO in the visible range and has an absorption wavelength in the 350 nm range, which aligns well with the solar radiation spectrum, and which makes these substrates valuable in the world of devices.

OPV photovoltaics highlight ongoing research endeavors aimed at tuning deposition parameters to further enhance the efficiency and applicability of these technologies [3]. Previous studies have shown that all nickel oxide (NiO) films produced on glass substrates using the sequential ionic adsorption method have a polycrystalline structure. In addition, there is a significant improvement in structural and crystalline properties compared to the base used to produce NiO films [4].Based on the importance and explanation of glass substrates, we will study indium tin oxide (ITO), fluorine tin oxide (FTO), and ordinary glass substrates.

Deposition

Despite the influence of the chosen substrates, purification and deposition conditions play the largest role in shaping the properties of coatings and films deposited on these substrates. During the past three decades, the successive ion layer adsorption and reaction (SILAR) method has emerged as one of the solution methods for depositing a variety of composite materials in the form of Thin layer [5].

One new solution method for thin film deposition is the sequential ion layer desorption and desorption (SILAR) method, which is also known as a modified version of chemical bath deposition[6].The sequential ion layer desorption and desorption (SILAR) method is based on Basic on the adsorption and reaction of ions from solutions during washing after each immersion in deionized water to prevent homogeneous precipitation in the solution. The basis of the SILAR approach is adsorption, which is the aggregation of one substance on the surface of another substance [5].The force of attraction between the ions in the solution and the surface of the substrate makes possible a surface phenomenon known as adsorption. The adsorption process is influenced by forces that can be cohesive, van der Waals, or chemoattractive, as well as other variables such as solution temperature, pressure, substrate type, solution concentration, substrate area, etc [1].

(1) Specific adsorption of the strongest ions of the chemical to be generated onto the substrate's surface happens when the substrate is submerged in the cationic precursor solution, (2) Rinse water to remove the excess solution as well as unadsorbed ions from the surface of the substrate , (3) upon subsequent immersion of the substrate in the anionic precursor solution a chemical reaction occurs between the well-adhering cations from the substrate surface and the anions in the precursor solution that form the desired compound [7].

Experimental Details

In this study, the production and characterization of NiO films on different substrates were carried out using the sequential ion layer adsorption and reaction (SILAR) method. The effect of the bases used in the SILAR technique used in the production of NiO films was investigated. In addition, the changes made by the base used on the physical and chemical properties of NiO films were determined.

Glass, FTO, ITO, and glass materials were used as the substrate for the growth of the films. The glass substrates were cut to 8 mm wide and 25 mm long. After the cutting process, the glass substrates, FTO, ITO, and glass were washed thoroughly with soapy water to get rid of dirt. After washing, the substrates were ultrasonically cleaned in acetone for 10 minutes. The clean FTO, ITO, and glass substrates were then dried in nitrogen gas. All operations were performed at room temperature and ambient pressure. Solutions were prepared to obtain nickel oxide layers by dissolving nickel (II) nitrate and aqueous ammonia in distilled water in a flask (one hundred milliliters) to obtain a ketone precursor and form compound ions ($[Ni(NH_3)_4]^{+2}$) with (pH≈10), where the reagents are used analytical for $NiCl_2$ and concentrated ammonia (NH_3) (28 %) are used to obtain a ketone precursor . The specific concentration values for a nickel (Ni) solution were 0.1 M and the molar ratio of Ni:NH_3 was 1:10 obtained as a result of several experiments. The SILAR growth cycle consists of four successive steps: (i) Dipping the substrate into the ($[Ni(NH_3)_4]^{+2}$) complex solution for 30 seconds to create a thin liquid film containing ($[Ni(NH_3)_4]^{+2}$) on the substrate; (ii) immediately dipping of the extruded substrates into hot water (90°C) for 7 seconds to form a NiO layer; (iii) dry the substrates in the air for 60 sec and (iv) then keep them in distilled water at room temperature for 30 minutes. Thus, the SILAR cycle is completed. The diagram showing the precipitation steps with the SILAR method to obtain nickel oxide films is shown in Fig1.

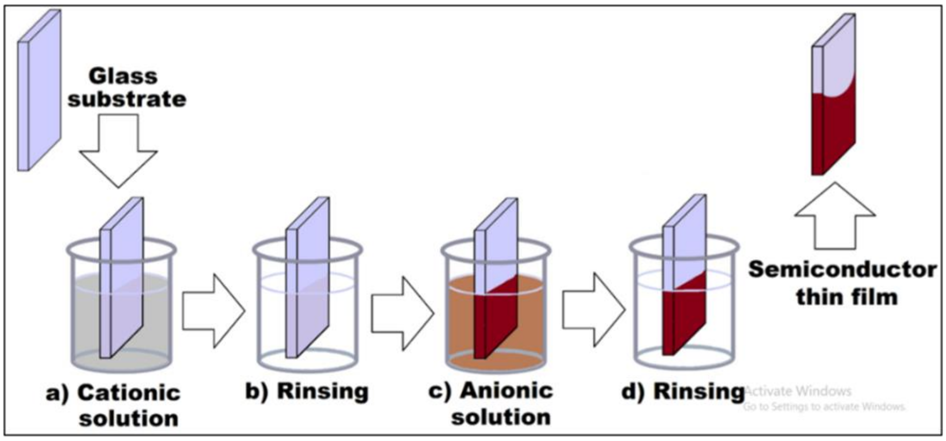

Fig. 1 Diagram representing the steps of sedimentation by the SILAR method to obtain Nickel Oxide films **.** [1]

Commercial nickel (II) nitrate was used, which is a solid substance with a green color and is commonly found in its aqueous form bound with water molecules in the form of hexahydrate.

The sedimentation cycle (SILAR) was repeated 40 times and the mass of nickel (II) nitrate to be added is determined by the following relationship

$$m = C \times M \times V \qquad (1)$$

C : molar concentration (mol/L)

V : solution volume (L)

M : The molar concentration of nickel (II) nitrate = 290.79 gm / mol

m : The mass of nickel (II) nitrate to be added to the solution (gm)

The process was repeated 40 times for all samples under the same conditions and annealing temperature of 600 K for 13 minutes in an ash furnace - annealing furnace.

Results and Discussion

Characterization (X-ray diffraction, UV-VIS, IV) of samples (NiO-ITO, NiO-FTO, NiO-Glass) of samples (NiO-ITO, NiO-FTO, NiO-Glass) and using the APD 2000 to obtain visual analysis and use PRO XRD device for analyzing X-ray results An X-ray diffractometer using 1.5405 angstroms (A°).

All XRD patterns to NiO-ITO, NiO-FTO, and NiO-Glass films are shown in Fig4. After examining them, it was determined that the material with the best crystallinity level of NiO films was NiO-ITO. NiO-Glass films have the lowest level of crystallinity compared to other films. While the crystallinity level of NiO-FTO films is worse than that of NiO-ITO films, it is better than that of NiO-Glass films. All films were determined to form in the cubic phase of NiO according to the Joint Committee on Powder Diffraction Standards card(JCPDS:01-073-1519) and the diffraction peaks were indexed depending on Fig 2. The diffraction peaks were found as a=b=c=4.165 A° for NiO-Glass films, a=b=c=4.157 A° for NiO-ITO films, and a=b=c=4.154 A° for NiO-FTO films. In addition, it was determined that the dominant growth in all films was in the (111), (200), and (220) Miller's indices directions respectively. On the other hand, when the spacing between crystals is obtained with the help of XRD patterns, the lattice parame ter of the cubic structure can be found by the following Equation (2).

$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad (2)$$

where h, k, and l are the Miller indices of the diffraction peak. Additionally, based on the full width at half maximum (FWHM) of a diffraction peak in X-ray diffraction (XRD) data, the average crystallite size (D) in a thin film can be estiamted by means of the Scherrer equation given as follow Equation (3).

$$D = \frac{0.9\,\lambda}{\beta \cos\theta} \qquad (3)$$

where D is the average crystallite size, λ is the wavelength of the X-rays, β is the FWHM of the peak in radians, and θ is the Bragg angle.[8]

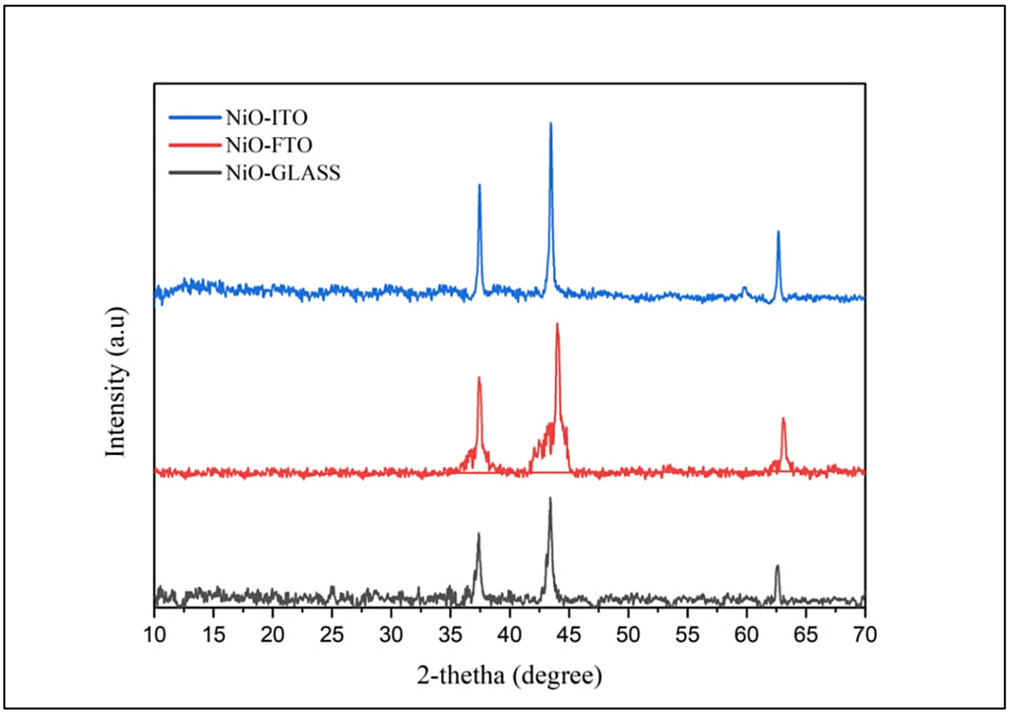

Fig.2 X-ray analysis of (NiO-ITO, NiO-FTO, NiO-Glass) films.

The texture coefficient (TC) is calculated by comparing the intensity of a particular diffraction peak (corresponding to a specific crystallographic plane) in the measured XRD pattern to the intensity that would be expected. The textrure coeffiecent gives Equation (4):

$$TC(hkl) = \frac{I_{(hkl)}/\ I_{0(hkl)}}{N^{-1}\sum_{N} I_{(hkl)}/I_{0(hkl)}} \qquad (4)$$

where I_{hkl} is the integrated intensity of the diffraction peak corresponding to the (hkl) plane, N is the number of the diffraction peaks, I_{0hkl} is the standard intensity of the level (hkl) taken from the (JCPDS) card.[8]

Depending on the previously mentioned equation and measurements obtained from UV-VIS Technique we can find energy gap by draw the relationship between ($\alpha h\nu$) and photon energy ($h\nu$) and by extending the straight line or tangent to the curve to the intersection of the photon energy axis at the point 0=($\alpha h\nu$), which represents the value of the energy interval, this satisfies the Tauc's Equation (5) (Eg=hν) and represents the energy interval results. [9]

$$\alpha h\nu = B(h\nu - E_g^{opt.})^b \qquad (5)$$

Based on the electronic transfers, Energy gap values can be determined. At (b=1/2) a direct transfer is considered permissible, while at (b=2) in the case of indirect transfers it is permissible.

Absorption coefficient (α) quantifies the ability of a material to absorb light at a specific wavelength. Mathematically, it can be expressed using Beer-Lambert's law as Depending on the results of UV-VIS to calculate the transmittance (T) and absorption (A) and the equations mentioned below .

$$\alpha = \frac{(-1)}{d} \mathrm{Ln}(T) \qquad (6)$$

Thus, the extinction coefficient is derived from the equation below.

$$k = \alpha\lambda/4\pi$$

Through the law of conservation of energy the reflectivity can be easily deduced from the equation below [10] .

$$T + R + A = 1 \qquad (7)$$

Optical Properties

Depending on UV-VIS results, some optical properties of pure nickel oxide deposited using a SILAR method on glass substrates (NiO-ITO, NiO-FTO, NiO-Glass) were calculated, which can be summarized in Table 1, also Some morphological properties are compared with the energy gap as shown in the Tables 2.

Table .1 Some resultes of optical properties of the films.

Simples	NiO-ITO	NiO-FTO	NiO-Glass
λ (nm)	300-950	300-950	300-950
Transmittance (T%)	30-54 %	17- 45 %	15-47 %
Absorption (A%)	53-28 %	77 -33 %	83-40 %
Reflectivity (R%)	17-22 %	6-20 %	2-20 %

Table.2 Structural Parameters with direct Energy gap.

Simples	Angle (2θ°)	FWHM (Radian)	Miller's Indices (hkl)	Grain Size (nm)	Energy Gap (eV)
NiO-Glass	43.39986	0.2908	200	29.39095	3.88
NiO-FTO	43.66393	0.260	200	32.857	3.84
NiO-ITO	43.48	0.290	200	29.421	3.81

The results showed that the transmittance values in the visible range of Nickel oxide films deposited by (SILAR) method on glass, substrates (NiO-ITO, NiO-FTO, NiO-Glass) increased gradually with wavelength and with clear contrast. In films deposited on (Glass substrate) , these bases showed somewhat linear behavior. Similar to the transmittance values, and although similar to the behavior of the films deposited on ITO and FTO, transmittance values of the films deposited on (ITO) were superior in transmittance, as shown in Fig 3.

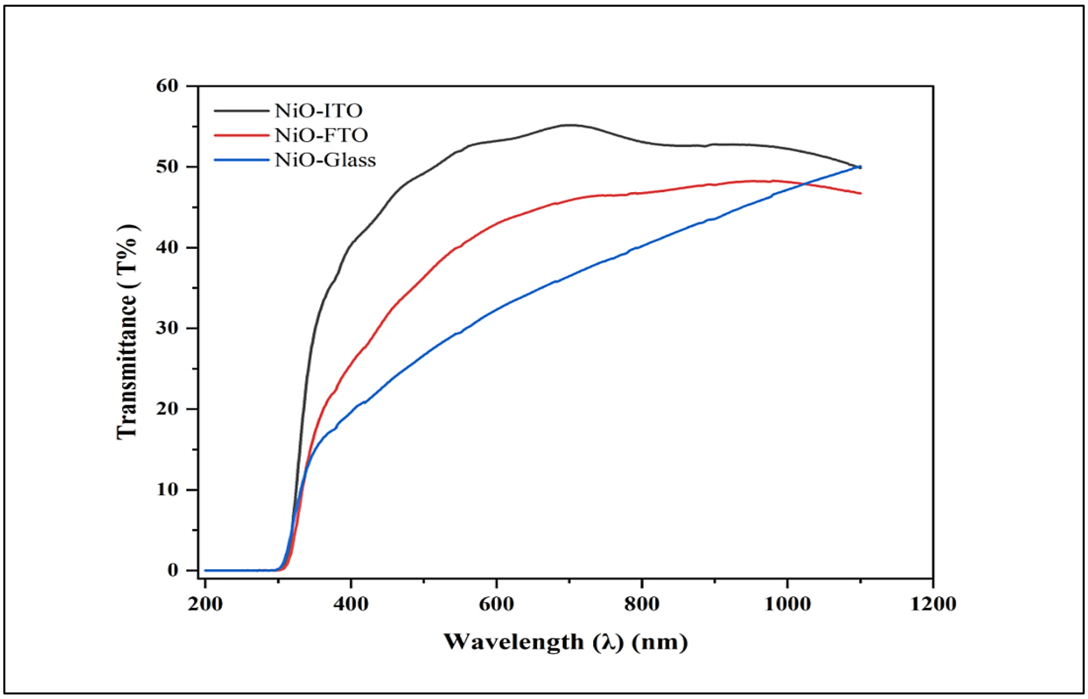

Fig. 3 Transmittance curve of films (NiO-ITO, NiO-FTO, NiO-Glass) withe wavelength.

The results showed that the absorption behavior for all samples is similar, with slightly different values, and that the maximum absorbance peaks are limited to a short range of wavelength (300-350 nm), and the absorbance values for all samples begin to decline in direct proportion to the energy, meaning that the absorbance values decrease with increasing wavelength, as shown in shapein Fig 4.

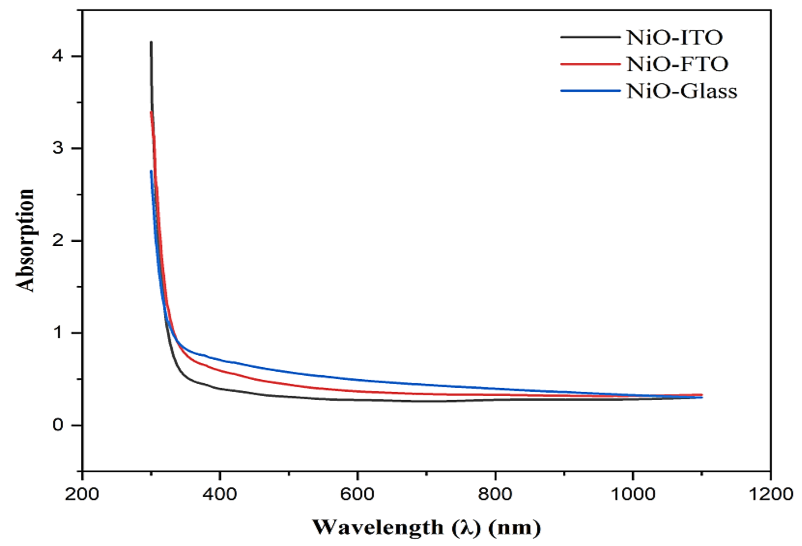

Fig. 4 Absorbance of (NiO-ITO, NiO-FTO, NiO-Glass) as a function of wavelength.

Absorption peaks occur in the wavelength range between 300 and 350 nm, indicating the presence of strong absorption in this wavelength range. This behavior could be due to several possible factors, including:

1. Effect of crystal structure The arrangement of atoms in the crystal lattice of nickel oxide films can have a significant impact on the absorption properties in this length range.

2. Electronic transition effects: This strong absorption may relate to electronic transitions within the electronic structure of the material, which occur at the mentioned wavelength.

3. Surface interactions There may be chemical reactions or surface interactions that occur in this length range, resulting in enhanced absorption in this range

The extinction coefficient measures a material's ability to absorb light at a specific wavelength, and is important for understanding how light interacts with films and how these properties affect application performance. Understanding the extinction coefficient helps us determine the amount of light absorbed by the film at a given wavelength, and this information can be used to design optical devices and improve their performance (Fig. 5) shows the absorption curve of nickel oxide films.

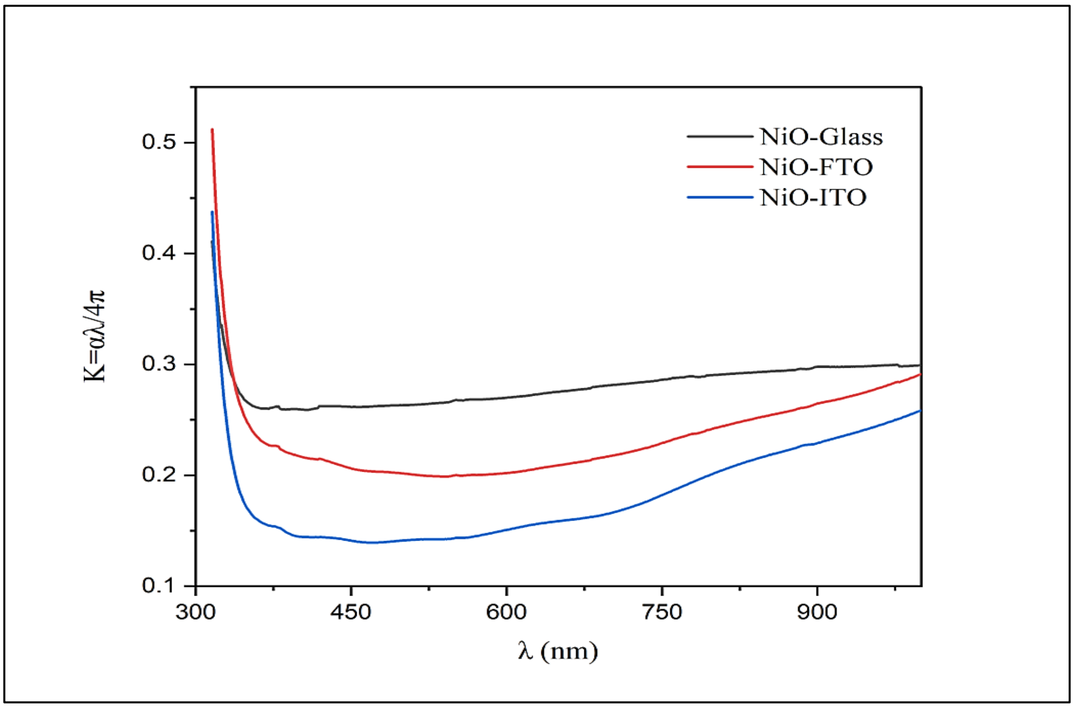

Fig. 5 Extinction coefficient of (NiO-ITO, NiO-FTO, NiO-Glass) as a function of wavelength .

Surface Interactions Differences in surface interactions between films and different glass substrates are responsible for the convergence of absorbance, extinction coefficient, and energy gap values. For example, surface interaction can lead to the formation of thin layers of different materials on the surface, which greatly affects the interaction of light with the system. In general, the presence of extinction factor peaks at a certain wavelength is a strong indicator of the interaction of light with the material studied in this range.

Fig 6 show the optical energy gap of NiO films for direct electronic transitions. The values of the direct optical energy gap were determined to be in the range of 3.81 - 3.88 eV.

The calculated band gap energy values for NiO films produced on ITO, FTO, and glass are 3.81, 3.84, and 3.88 eV, respectively. The Energy gap values of NiO films produced on ITO and FTO substrates are almost the same. However, Energy gap values of (NiO) films produced on glass are higher than those of films produced on other substrates. NiO films produced on glass substrates have the largest band gap (3.88 eV) for direct band transition.

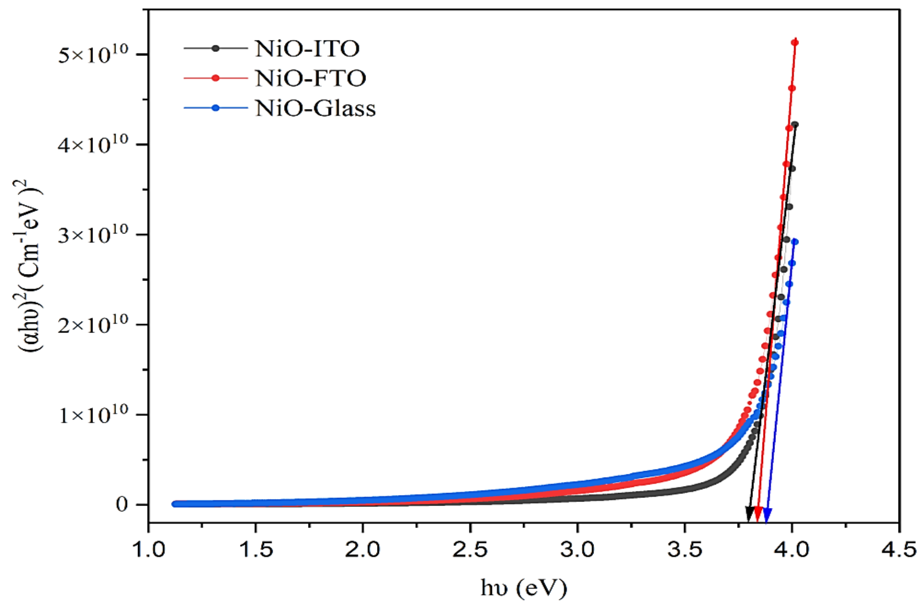

Fig.6 Direct Energy gap of (NiO-ITO,NiO-FTO and NiO-Glass).

The calculated energy gap values roughly agree with the values measured in various studies of nickel oxide films. This indicates that the technique used for film deposition is considered a good standard for measuring the various films to be studied. However, it should be noted that these values are highly dependent on the experimental conditions and methods used to prepare the membranes, and these values should be confirmed using appropriate analytical techniques in each specific case.

Conclusions

- (NiO) films deposited using the SILAR method on various glass substrates (ITO, FTO, glass) exhibit different optical properties.
- Transmittance values in the visible range increase gradually with wavelength, showing a clear superiority in films deposited on ITO substrates.
- Absorption behavior is similar across all samples, with slightly different values, with maximum absorbance peaks limited to a short wavelength range (300-350 nm).
- The absorbance values decrease proportionally with increasing wavelength, indicating a consistent trend across the samples .
- The calculated energy gap values (ranging from 3.91 to 3.97 eV) roughly agree with those measured in other studies, suggesting the reliability of the SILAR method for film deposition and characterization .
- These findings contribute to understanding the optical properties of Nickel Oxide films deposited on different glass substrates and highlight the potential of the SILAR method for such applications.

Based on the results above, the potential applications of these films could include:

The possibility of using films deposited on ETO substrates in optoelectronic devices as transparent conductive coatings, solar cells, touch screens and display screens due to their high transmittance values.

The ability to absorb a wide range of rays, especially ultraviolet rays, makes it possible for these films to have applications to protect against ultraviolet rays, such as window coatings or lenses to prevent harmful ultraviolet rays.

The energy gap calculated for all samples and their absorbance in the visible range is considered a good ability to convert energy and can be used in developing photovoltaic devices such as solar cells, touch screens, etc.

All films deposited, especially on regular glass substrates, were characterized by a gradual increase in transmittance over the wavelength range, which raises the possibility of their application in anti-reflective coatings and improving optical systems.

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تأثير أنواع الركائز على الخواص البصرية لأغشية أوكسيد النيكل (NiO) المترسبة بطريقة امتزاز وتفاعل الطبقة الايونية المتسلسلة (SILAR)

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الخصائص البصرية، الركائز الزجاجية،اغشية اوكسيد النيكل ، FTO، ITO، فجوة الطاقة، معامل الانكسار، SILAR.

معلومات المؤلف

الخلاصة:

في هذه الدراسة تم تشخيص بعض الخواص البصرية لأغشية أوكسيد النيكل (NiO) المترسب على ركائز زجاجية مختلفة (ITO، FTO، زجاج) بطريقة امتزاز وتفاعل الطبقة الأيونية المتسلسلة (SILAR). تم تحديد جميع الأفلام لتشكل في الطور المكعب من NiO وفقًا لبطاقة اللجنة المشتركة المعنية بمعايير حيود المسحوق (JCPDS:01-073-1519). تم قياس بعض الخصائص البصرية مثل فجوة الطاقة حيث تغيرت قيم فجوة الطاقة الضوئية المباشرة في المدى (3.81- 3.88 eV). أظهرت النتائج أن قيم النفاذية في المدى المرئي للعينات تزداد تدريجياً مع الطول الموجي (من 15% إلى 54%)، مع تفوق واضح في قيم النفاذية للأغشية المودعة على ركائز ITO. وعلى غرار قيم النفاذية والامتصاصية للعينات، أظهرت الأفلام المودعة على (الزجاج) سلوكاً خطياً، على عكس بقية العينات المودعة على ركائز FTO وITO، والتي أظهرت سلوكاً أسياً مع نفاذية أعلى. ولوحظ سلوك مماثل لامتصاص الضوء في جميع العينات، مع انخفاض متناسب في قيم الامتصاص مع زيادة الطول الموجي. وكانت نتائج الأفلام مطابقة بشكل تقريبي للدراسات السابقة مما يدل على موثوقية طريقة SILAR في تحضير الفيلم وتوصيفه. تقتصر قمم الامتصاص القصوى على مدى الطول الموجي القصير (300-350 نانومتر).