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Structural and Optical Properties of Nickel Oxide Thin Films Deposited by Sol-Gel Dip-Coating Technique

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Abstract

In this research, pure nickel oxide (NiO) nano-thin films were prepared by sol-gel technique using dip deposition method on glass substrates at 100°C. The structural properties of all prepared thin films were studied using X-ray diffraction (XRD) technique, while the optical properties of the prepared films were studied using UV-Vis spectroscopy. The XRD results showed that the nickel oxide films have a cubic polycrystalline structure and that the predominant crystallization direction is (111). The interplaner distance for all peaks and the lattice constants were calculated, and these values were found to be in agreement with the International Standards Card for NiO. The crystallite size of the films prepared at 100°C was 23.97 nm, and the dislocations and number of crystals per unit area were also calculated. The optical properties of the prepared films were studied by recording the transmittance and absorbance spectra over the wavelength range (300-800) nm. The optical properties results showed that the light transmittance of the films increases with increasing wavelength by (>90%) in the visible light region and near the infrared region, and the absorbance decreases with increasing wavelength and that the absorption edge is located at 360 nm with an absorption energy of about (3.44 eV). The results obtained from the (NiO) films indicate that it is a semiconductor with a wide optical energy gap of (3.61eV).

Key words: Nanomaterials, Semiconductor, Optical properties, Structure properties, Sol-gel.



الخصائص البنيوية والبصرية لأغشية أكسيد النيكل الرقيقة المترسبة بتقنية طلاء الغمس بالمحلول الهلامي

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الملخص

في هذا البحث، تم تحضير أغشية نانوية رقيقة من أكسيد النيكل النقى (NiO) بتقنية المحلول الهلامي باستخدام طريقة الترسيب بالغمس على ركائز زجاجية عند درجة حرارة 100 درجة مئوبة. دُرست الخصائص البنيوبة لجميع الأغشية الرقيقة المُحضرة باستخدام تقنية حيود الأشعة السينية (XRD)، بينما دُرست الخصائص البصرية للأغشية المُحضرة باستخدام مطيافية الأشعة فوق البنفسجية-المرئية. أظهرت نتائج حيود الأشعة السينية أن أغشية أكسيد النيكل لها بنية مكعبة متعددة البلورات وأن اتجاه التبلور السائد هو (111). حُسبت المسافة بين المستوبات لجميع القمم وثوابت الشبكة، ووجد أن هذه القيم تتفق مع بطاقة المعايير الدولية لأكسيد النيكل. بلغ حجم بلورة الأغشية المُحضرة عند درجة حرارة 100 درجة مئوية 23.97 نانومتر. دُرست الخواص البصرية للأغشية المُحضرة من خلال تسجيل أطياف النفاذية والامتصاصية على مدى الطول الموجى (300-800) نانومتر. أظهرت نتائج الخواص البصرية أن نفاذية الضوء للأغشية تزداد بزيادة الطول الموجى بنسبة (>90%) في منطقة الضوء المرئي وبالقرب من منطقة الأشعة تحت الحمراء، وأن الامتصاصية تقل بزيادة الطول الموجى، وأن حافة الامتصاص تقع عند 360 نانومتر مع طاقة امتصاص تبلغ حوالي (3.44 إلكترون فولت). تشير النتائج التي تم الحصول عليها من أغشية أكسيد النيكل (NiO) إلى أنها شبه موصل بفجوة طاقة بصربة واسعة تبلغ (3.61 إلكترون فولت).

الكلمات المفتاحية: مواد نانوية، أشباه موصلات، الخواص البصرية، الخواص التركيبية، المحلول الهلامي.

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1. Introduction:

Materials are classified based on the energy band theory into three types: conductor, insulator, and semiconductor. In a conductor, there is an overlap between the conduction band (CB) and the valence band (VB), which allows the free movement of electrons, while insulators have a large forbidden band with a value of about (5 eV) called the energy gap (Eg), in which electrons cannot move unless they acquire sufficient energy equal to or greater than their energy gap [1].

Oxide semiconductors have made significant progress over the past decade, gaining widespread use across a range of electronic devices, including thin-film transistors, photovoltaics, light-emitting diodes, sensors, non-volatile memory devices, and catalysts, among many other applications. In particular, the resilience of oxides' electronic properties against mechanical deformation or degradation during operation under ambient conditions, as well as the ability to process oxides at low temperatures, has made them the preferred materials for flexible electronics based on polymers, cellulose, and flexible substrates [2]. P-type oxides are of great importance for a wide range of emerging applications, including transparent metal oxide semiconductors for integrated circuits, hole-transporting layers for photovoltaics, and flexible p-n junctions. Three of the most common p-type oxides are tin monoxide (SnO), copper oxide (Cu₂O), and nickel oxide (NiO) [3, 4].

Nickel oxide (NiO) has become widely known and plays an important role in various research areas such as science, technology, medicine, and renewable energy [2]. Nickel oxide belongs to the II-VI family of semiconductors. However, the crystal structure of nickel oxide is cubic [5-7]. Several methods have been used to manufacture NiO films, such as thermal decomposition [8], sputtering [9], and solution-gelling [3]. Sol-gel method is preferred by researchers due to its great advantages such as simple preparation method, low equipment, and low preparation temperature [10-13].

In this study is to examine the preparation of pure nickel oxide thin films using the sol-gel method and the method of depositing metal oxide films, as well as the use of inspection methods to determine the structural and optical properties of the manufactured films

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deposited on a glass substrate; thus, the possibility of benefiting from the properties of the synthesized films in electro-optical applications and solar cells.

2. Materials and Methods

Preparation of pure NiO nano-thin film samples using the sol-gel dip-coating technique. NiO nano-thin films were prepared from a nickel chloride solution (NiCl₂.6H₂O) with a molar mass (M) of 237.69 g/mol. To prepare the NiO films, nickel chloride was used with a purity of 99.5%. It is a green powder that is readily soluble in water. The solution was prepared at room temperature and at a concentration of 0.1 M. This was done by dissolving 1.745 g of nickel chloride in 80 ml of distilled water. It was then stirred on a magnetic stirrer for a one an hour, until a clear, homogeneous solution was obtained. The solution was then stored in a Becker glass and left for 24 hours at room temperature to ensure homogeneity and to ensure the absence of precipitates or suspended particles. It was then left to form a gel [14,15].

- **2.1 Thin Film Deposition:** After completion After 24 hours, the solution is homogenized and no sediments or suspended solids remain. The sedimentation process begins with several steps:
- i. The glass substrate is fixed vertically with a tool.
- ii. The substrate is immersed in the gel for 30 seconds.

The glass substrate is placed on a hot plate at 100°C for 5 minutes to evaporate and dry the thin layer, resulting in thin films attached to glass substrates [15].

3. Results and Discussion

3.1 Structural Results

The results of the structural properties analysis of pure NiO thin films prepared at 100°C, obtained using X-ray diffraction (XRD), showed that they had a cubic (polycrystalline) structure, as shown in Fig. 1(a). This is consistent with the results of previous studies. [4-7] the resulting curves were analyzed using Origin Pro24b software to accurately determine the locations of the X-ray diffraction peaks of the thin films, as shown in Fig. 1(b). These peaks appear sharply when X-ray beams are irradiated at different



angles on the film, allowing them to constructively interfere under Bragg's law. Fig. 1, shows the analysis of the data obtained from the XRD. By analyzing the curves, we notice the appearance of several peaks, all of which are related to NiO, and we notice that the prevailing direction of growth is (111). The structural parameters [hkl, 20 $_{\text{Max}}$, dhkl, β , and D] were then calculated, as shown in Table (1). It was also found that these results are somewhat consistent with the international standard card (Joint Committee of Powder Diffraction Standards) with the number (JCPDS04-0835), and this is consistent with the results of scientific studies [5-7].

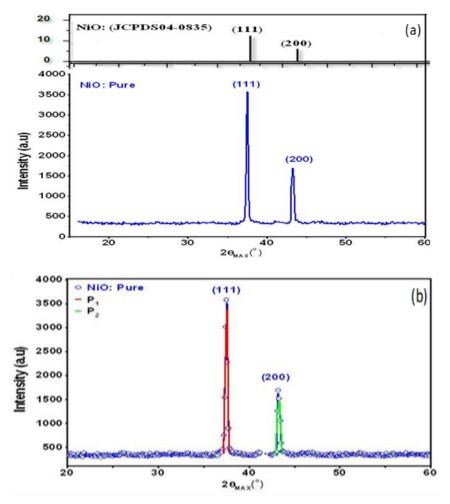


Fig. 1: X-ray diffraction patterns of a pure NiO film in (a), (b) XRD data analysis using Origin Pro24b software, for a pure NiO thin films. Film deposited by sol-gel dip-coating technique.



Table (1): Shows some structural results obtained from XRD of pure nickel oxide (NiO) films compared with card (JCPDS04-0835).

| Samples | Interplaner distance (hkl) | 20Max (degree) | d _{hkl} (A ^o) | FWHM β(rad) | Average crystalline size [Dav(nm) |
|-----------|-------------------------------|-------------------|------------------------------------|----------------|-----------------------------------|
| NiO: Pure | (111) | 37.473 | 2.399 | 0.00611 | 23.9691 |
| | (200) | 43.297 | 2.088 | 0.00916 | 16.2872 |
| NiO: | (111) | 37.280 | 2.410 | | |
| (JCPDS) | (200) | 43.250 | 2.091 | | |

3.2 Results of Optical Measurements:

The spectra obtained from pure nickel oxide thin films are shown in Fig. 2 (a, b). Fig. 2(a), shows an increase in transmittance with increasing wavelength. Furthermore, the NiO thin films exhibit transmittance (>90%) in the visible light range and in the near-infrared. Additionally, a sharp increase in transmittance can be observed in the range (320–450 nm) [8]. Therefore, the fundamental absorption edge can be identified, and it appears to have shifted to higher photon energy in the form of a curve. This shift to higher energies proves that the NiO thin film is a semiconductor with a wide energy band gap, while the curved shape confirms that the NiO thin film is a cubic polycrystalline structure.

Fig. 2(b), shows changes in the transmittance and absorbance spectra, respectively, as a function of photon wavelength. Figure 1 indicates that the absorbance decreases with increasing wavelength of the incident photon. Although the maximum absorbance is obtained in the range (300-800 nm), the energy of the incident photon cannot excite the valence band electron to the conduction band, as its energy is about (2.18 eV), which is less than the optical energy gap [8].



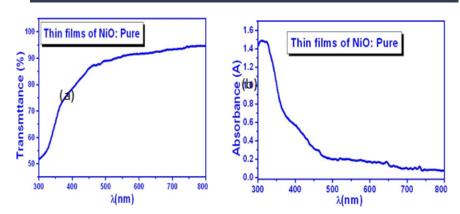


Fig. 2: (a) Shows the change in transmittance, (b) represents the change in absorbance; as a function of wavelength for a pure NiO film. Films deposited by sol-gel dip-coating technique.

The optical energy band gap, which is defined as the electron excitation energy from the top of the valence band to the bottom of the conduction band, for the allowed direct electronic transitions can be determined by plotting the relationship between $(\alpha h v)^2$ and (h v) according to the Tuck equation [15]. Fig. 3, shows a graph of $(\alpha h v)^2$ versus photon energy (h v) for a pure nickel oxide thin film. As shown, the optical energy gap is 3.61 eV.

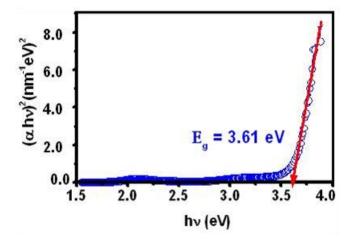


Fig. 3: Shows the value of the optical energy gap for the direct transition allowed for the pure NiO thin film deposited by sol-gel dip-coating technique

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4. Conclusion:

We successfully prepared nickel oxide (NiO) nano- thin films using the sol-gel dip-coating technique. This research demonstrated that XRD analysis of all films showed that they were cubic polycrystalline, and optical properties analysis results revealed that increasing the wavelength leads to increased transmittance and, on the other hand, decreased absorbance. The film's transmittance is extremely high, exceeding 90% in the visible and infrared light range. This makes nickel oxide a good candidate for many future medical and allergic applications, as well as photovoltaic, optoelectronic, and lithium-ion battery applications. The pure NiO thin film has been proven to be a semiconductor with a wide optical energy band gap of 3.61 eV.

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