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Studying Some Optical Properties of Magnesium Oxide by Depending on Different Thicknesses

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دراسة بعض الخواص البصرية لأوكسيد الماغنسيوم اعتماداً على سماكات مختلفة

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Abstract:

This study investigates the optical properties of magnesium oxide (MgO) thin films with different thicknesses (16, 24, and 36 nm) using a UV–Vis spectrophotometer (Min 1240). The absorbance spectra showed a similar behavior for all samples, with a sharp increase around 460 nm, and higher absorbance values for thinner films. The transmittance spectra revealed a decrease with decreasing thickness in the wavelength range of 382–487 nm. The absorption coefficient (α) was calculated and found to be greater than 6.64×10^4 cm^{-1}, indicating direct electronic transitions. The optical Energy gap (Eg) was determined using the Tauc method and found to be 2.558 eV. A slight decrease in Eg with increasing thickness was observed, attributed to structural changes, including reduced defect density and grain-boundary effects.

Keywords: Magnesium oxide, Thicknesses, Optical properties, Absorbance, Transmittance, Absorption coefficient, Energy gap.

الملخص:

تتناول هذه الدراسة الخواص البصرية لأغشية أكسيد المغنيسيوم (MgO) الرقيقة بسماكات مختلفة (16، 24، 36 نانومتر) باستخدام مطياف الأشعة فوق البنفسجية–المرئية (UV–Vis) من نوع Min 1240 أظهرت أطياف الامتصاص سلوكًا متشابهًا لجميع العينات مع زيادة حادة عند الطول الموجي 460 نانومتر، كما زادت قيم الامتصاصية مع انخفاض السمك. أوضحت أطياف النفاذية انخفاضها مع نقصان السمك ضمن المدى (382–487 نانومتر). تم حساب معامل الامتصاص (α) ووجد أنه أكبر من 6.64×10^4 سم$^{-1}$، مما يدل على انتقالات إلكترونية مباشرة. كما تم حساب فجوة

الطاقة البصرية (Eg) باستخدام طريقة تاوك، وبلغت قيمتها 2.558 إلكترون فولت. ولوحظ انخفاض طفيف في فجوة الطاقة مع زيادة السمك، ويُعزى ذلك إلى التغيرات التركيبية مثل انخفاض كثافة العيوب وحدود الحبيبات.

الكلمات المفتاحية: أكسيد المغنيسيوم، السماكات، الخصائص البصرية، الامتصاص، النفاذية، معامل الامتصاص، فجوة الطاقة.

1. Introduction:

1.1. Magnesium oxide:

Magnesium oxide (MgO) is considered an ideal model for simple ionic oxides that adopt a rock-salt (Face-Centered Cubic) crystal structure [1]. This stable configuration confers exceptional physical properties on the compound, most notably a melting point of 2,852°C, making it a strategic material for industrial refractory applications [2].

From an electronic perspective, MgO is classified as a wide bandgap insulator with an energy gap of approximately 7.8 eV. This characteristic provides it with high optical transparency across the ultraviolet and visible spectra [3]. Due to its chemical stability and strong ionic bonding, magnesium oxide is widely used as a primary substrate for the growth of superconducting thin films and magnetic oxides [4].

In modern research, studies have demonstrated that nano-crystalline magnesium oxide (MgO nanoparticles) synthesized via the sol-gel method possesses a high surface area and advanced optical properties. These features open new horizons in chemical catalysis and optical sensing [5].

2. Theoretical background:

2.1. Optical Properties:

"The study of optical properties of solids has a vital role in revealing the band structure of materials for use in optical and electronic devices. These properties are highly dependent on the chemical composition of the host material.") [22].

2.1.1. Absorbance:

Absorbance is defined as "the logarithm of the ratio of incident to transmitted radiant power through a sample (excluding the effects on cell walls)"[21]. Absorbance (A) is a dimensionless physical quantity that expresses the amount of light absorbed by a material as electromagnetic radiation passes through it. In solid-state physics, the study of absorbance is of paramount importance for understanding the interactions between photons and electrons, as it is directly related to the absorption coefficient ($\propto$), which determines the material's opacity or transparency to specific radiation [6].

This phenomenon is governed by the Beer-Lambert Law, which states that absorbance is directly proportional to the concentration of the absorbing species and the optical path length. In the case of oxides such as Magnesium Oxide (MgO), optical absorbance measurements in the Ultraviolet-Visible (UV-Vis) range are utilized to determine the material's optical bandgap. A sharp increase in absorbance, known as the absorption edge, occurs at specific energy levels representing the transition of electrons from the valence band to the conduction band [7].

Furthermore, absorbance spectra serve as a critical diagnostic tool for detecting crystal defects and impurities. These irregularities manifest as additional absorption bands in spectral regions where the pure material is typically transparent. Consequently, absorbance spectroscopy is a highly effective, non-destructive analytical method for evaluating the quality and electronic structure of synthesized nanomaterials [8].

2.1.2. Transmittance:

Transmittance (T) is defined as the effectiveness of a material in transmitting radiant energy; it is the ratio of the radiant flux transmitted by a body to that incident upon it [9]. In solid-state physics and materials science, transmittance spectra are essential for characterizing the optical window of insulators and semiconductors. For wide-bandgap oxides such as Magnesium Oxide (MgO), high transmittance in the visible spectrum is a hallmark of high crystalline quality and stoichiometry [10].

Experimental measurement of transmittance allows researchers to determine the extinction coefficient and the refractive index of thin films. Furthermore, the relationship between transmittance and sample thickness is fundamental to applying the Beer-Lambert Law for quantitative analysis [11]. In the infrared region, transmittance dips are used to identify vibrational modes of the crystal lattice (phonons) and the presence of adsorbed species on the material surface [12].

2.1.3. Absorption coefficient:

The absorption coefficient is a fundamental material property that characterizes the rate of decrease in the intensity of electromagnetic radiation as it propagates through a medium [13]. It is an intrinsic parameter that depends on the material's chemical composition, crystal structure, and the frequency of the incident radiation. In the field of optical characterization, it serves as the link between macroscopic measurements (like absorbance) and microscopic electronic transitions [14].

For wide-bandgap metal oxides, such as Magnesium Oxide (MgO), the absorption coefficient remains near zero throughout the visible spectrum but increases sharply (often exceeding 10^4 cm^{-1}) at the fundamental absorption edge in the ultraviolet region [15]. This rapid increase corresponds to the transition of electrons from the valence band to the conduction band. Accurately determining is essential for calculating the optical conductivity and the extinction coefficient (k), which are vital for designing optoelectronic devices and protective coatings [16].

2.1.4. Energy gap:

an electron from the top of the valence band to the bottom of the conduction band [17]. This fundamental parameter dictates the optical and electrical behavior of materials. Materials with a wide bandgap, such as Magnesium Oxide ($E_g \approx 7.8\,eV$ function as transparent insulators in the visible spectrum, whereas narrow-bandgap materials interact more dynamically with various light frequencies [18].

Experimentally, the energy gap is determined by analyzing the absorption coefficient (α) using Tauck's Relation, where a plot of $(\alpha h\nu)^{1/n}$ versus photon energy ($h\nu$) is generated. The value of the exponent n depends on the nature of the electronic transition—whether it is a direct or indirect transition [19]. Controlling and "tuning" the energy gap, particularly in nanomaterials, is crucial for advancements in photovoltaic cells, optical sensors, and UV-protective coatings [20].

3. Research problem:

There is a need to understand how the thickness of MgO thin films affects their optical properties, particularly absorbance, transmittance, absorption coefficient, and optical band gap. These properties are critical for applications in optoelectronic devices, yet their dependence on thickness is not fully clarified.

4. Objective:

1-To study the effect of film thickness on the optical properties of MgO thin films.
2-To analyze absorbance and transmittance behavior at different wavelengths.
3-To calculate the absorption coefficient (α) of the films.
4-To determine the optical band gap (Eg) using the Tauc method.
5-To investigate the relationship between thickness and electronic transitions.

5. Importance of the Research:

1-MgO is widely used in optoelectronic and optical coating applications.
2-Understanding its optical behavior enhances its performance in devices such as sensors and solar cells.
3-The study provides insight into how thickness influences material properties, which is important for thin film engineering and nanotechnology.

6. Materials, Devices, and Tools:

Material: Magnesium Oxide (MgO) thin films.
Thicknesses: 16 nm, 24 nm, 36 nm.
Device: UV–Vis spectrophotometer (Min 1240), A computer with all accessories.
Tools: Film deposition system, thickness measurement tools.

7. Methodology:

1-MgO thin films were prepared with different thicknesses (16, 24, and 36 nm).
2-Optical measurements were carried out using a UV–Vis spectrophotometer in the wavelength range of 382–487 nm.
3-Absorbance and transmittance spectra were recorded.
4-The absorption coefficient (α) was calculated using the relation:

$$\alpha = \frac{2.303A}{t}$$

5-The optical band gap (Eg) was determined using the Tauc plot method by plotting $(\alpha h\nu)^2$ versus photon energy (hν).
6-The linear region was extrapolated to obtain Eg.

8. Results and Discussion:

Thin metal oxides, such as magnesium oxide (MgO), are very important in optical and electronic applications due to their unique properties, including absorption and light transmission. Studying the effect of film thickness on these properties helps elucidate how light propagates through the material and how to improve the performance of electronic and optical devices.

In this study, MgO films of different thicknesses (16, 24, and 36 nm) were investigated using a UV-Vis spectrophotometer. The focus was on measuring absorbance, light transmission, and the absorption coefficient to determine their relationship with film thickness. The optical energy gap (Eg) was also calculated to evaluate the effect of thickness on the electronic properties of the films.

These results help clarify how changes in grain size and crystalline structure of the films affect light behavior and electron transitions, which is important for the development of devices such as sensors, optical insulators, and thin-film electronics.

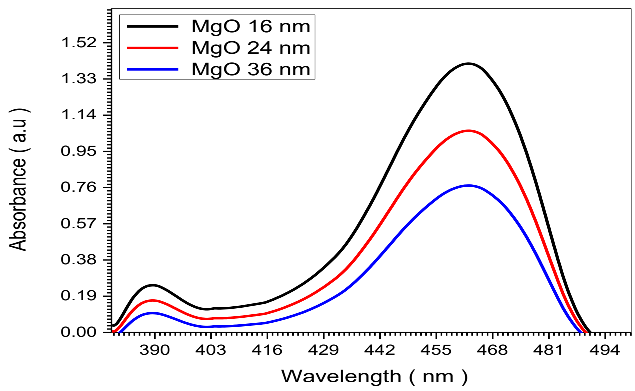

Figure (1) Relationship between absorbance and wavelength of MgO samples with different thicknesses (16, 24, and 36) nm

The relation between absorbance and wavelengths, we found that the behavior of curves is the same for all samples of MgO with different thicknesses (16, 24, and 36) nm studied using a UV-VS min 1240 spectrophotometer. Show all results of absorbance in Figure1. In figure1 shows the relation between absorbance and wavelengths, with the rapid increase of the absorption in the wavelength (460 nm). The effects of the thickness of samples, the absorbance value increased with the decrease

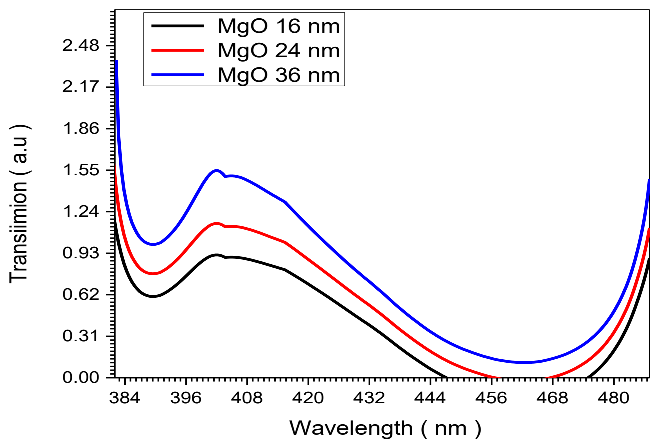

Figure (2) relationship between transmittance and wavelength of MgO samples with different thicknesses (16,24 and 36) nm

Figure (2) shows the tr transmittance, and we have discussed in this section the range (382 to 487 nm). From figure (2), the transmittance spectra (decrease) from the sample MgO with different thicknesses (16,24 and 36) nm, and the curves reach saturation above 460 nm, and the average transmittance of the samples is 1.55 (a.u)

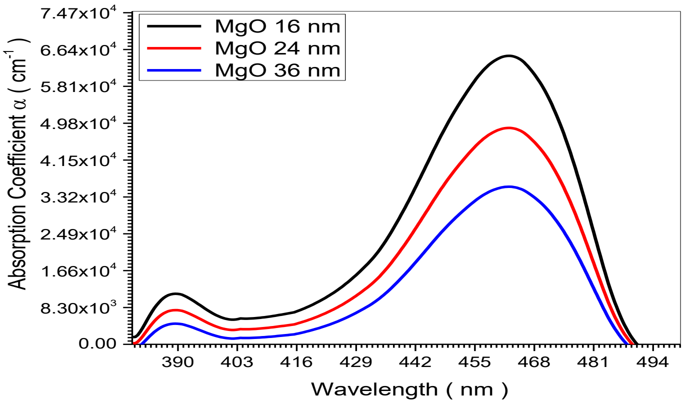

Figure (3) Relationship between Absorption coefficient and wavelength of MgO samples with different thicknesses (16, 24, and 36) nm

The absorption coefficient (α) of the prepared MgO samples with different thicknesses (16, 24, and 36) nm was found from the following relation: α = 2.303 A/t Where (A) is the absorbance and (t) is the film thickness. Figure (3) shows the plot of (α) with wavelength (λ), which shows that the value of $\alpha > 6.64 \times 10^{\wedge}4\ cm^{-1}$ for all films in the visible region. This means that the transition must correspond to a direct electronic transition, and the properties of this state are important, since they are responsible for electrical conduction. Also, figure 3 shows that the value of (α) for the sample 16 nm is greater than that of the sample 36 nm. The decrease in absorbance coefficient is due to the increase in grain size and decrease in the number of defects.

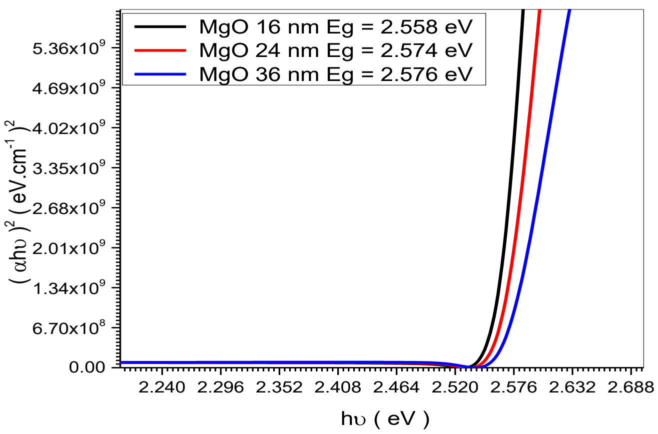

Figure (4) the optical energy gap (Eg) of MgO samples with different thicknesses (16, 24, and 36) nm

The optical energy gap (Eg) has been calculated by the relation $(\alpha h\upsilon)^2 = C\,(h\upsilon - Eg)$ Where C is a constant. By plotting $(\alpha h\upsilon)^2$ vs photon energy (hυ) as shown in figure (4). And by extrapolating the straight thin portion of the curve to intercept the energy axis, the value of the energy gap has been calculated. The value of (Eg) obtained was (2.558) eV, which approaches the value of (2.574) eV reported elsewhere [3]. The value of (Eg) was decreased from (2.574) eV to (2.558) eV at different thickness increases. The decreasing of (Eg) may be related to a decrease in grain boundaries and their density due to the heating effect of the polycrystalline thin films. It was observed that the different structures of the samples with different thicknesses confirmed the reason for the band gap shifts.

9. Recommendations:

1-Study a wider range of thicknesses for more accurate analysis.
2-Investigate the effect of temperature on optical properties.
3-Use additional characterization techniques such as XRD or SEM to study structure.
4-Explore the application of MgO films in solar cells and optical devices.
5-Improve film preparation methods to reduce defects and enhance performance.

10. Conclusion:

The optical properties of MgO thin films are strongly dependent on film thickness. Thinner films exhibit higher absorbance and absorption coefficients, while transmittance decreases. The absorption coefficient values indicate direct electronic transitions. The optical band gap was found to decrease slightly with increasing thickness, likely due to structural improvements such as reduced defects and grain boundary density. These findings highlight the importance of thickness control in optimizing MgO thin films for optical and electronic applications.

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