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Research Article

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Exploring the Optical Properties of ZnO Thin Films on Sapphire Substrates

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Abstract: This study investigates the optical properties of zinc oxide (ZnO) thin films deposited on sapphire substrates, emphasizing their relevance in optoelectronic applications. The theoretical analysis focuses on determining the reflection and transmission coefficients for a ZnO layer in relation to air and when combined with sapphire. We found that over the entire wavelength range studied, the transmission of sapphire is superior to that of ZnO, with a maximum value of 0.92 or 92% for sapphire and 0.89 or 89% for ZnO. This is explained by the fact that sapphire is transparent up to 8.8 eV, corresponding to its energy band, whereas ZnO is transparent up to just 3.3 eV, corresponding to its gap. A very large value of a material's transmission can depend on its surface. Additionally, the study examines the impact of film thickness on the optical properties of the ZnO/sapphire system. Increased thickness leads to enhanced interference effects, with reflection and transmission varying significantly. Notably, the maximum transmission recorded for the ZnO/sapphire system is 92%, while reflection drops to 8% within the 400-1000 nm range. However, the crystalline quality of ZnO still requires improvement due to a high defect density at the interface, which affects overall performance. The results underscore the critical role of both the ZnO layer and the sapphire substrate in optimizing optical transmission. Effective coatings combining these materials can significantly enhance the performance of optoelectronic devices, making them valuable for future technological applications.

Keywords: Zinc Oxide, sapphire, reflection, transmission, substrate

1. Introduction

The study of the ZnO/sapphire system has garnered significant interest among researchers due to the intriguing optical properties of these two materials, which can be applied in various technological domains. Zinc oxide (ZnO) is classified as a transparent conductive oxide (TCO) and is distinguished by its wide bandgap of 3.37 eV, allowing it to be transparent to visible and infrared radiation. Furthermore, ZnO exhibits a substantial excitonic binding energy of 60 meV [1-2], making it an attractive candidate for optoelectronic applications such as light-emitting diodes (LEDs) and solar cells. Its diverse properties support applications in piezoelectric transducers [3] and gas sensors [4], enhancing its relevance in modern technology. Sapphire, chemically represented as Al_2O_3 (aluminum oxide), is an ionic insulating crystal known for its remarkable mechanical, chemical, and thermal properties [5]. It has historically been utilized in the growth of gallium nitride (GaN) since 1969 [6] and continues to play a crucial role in the fabrication of advanced optoelectronic devices. Sapphire's bandgap of approximately 8.8 eV, while affected by various crystalline defects [7-12], contributes to its excellent optical transmission characteristics across a wide range of wavelengths. This makes sapphire suitable for applications in laser technology, high-quality imaging systems, and mobile devices. This theoretical study focuses on the optical properties of the ZnO/sapphire interface, specifically analyzing the reflection and transmission coefficients. This study aims to provide a comprehensive understanding of the optical interactions within the ZnO/sapphire system, highlighting its significance for future technological innovations.

I- Theoretical Study

When a wave hits a surface separating two media with different refractive indices, it is partially reflected and partially transmitted.

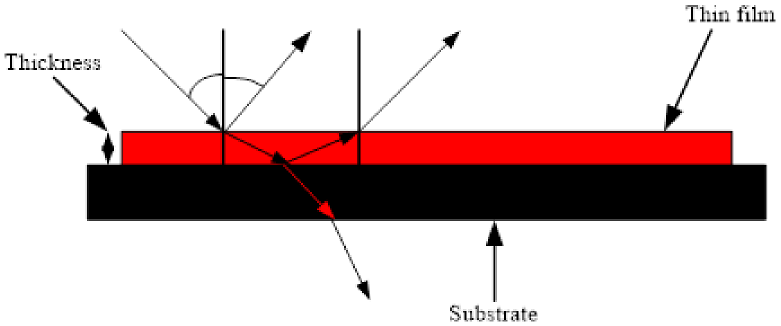

Figure 1: Illustration of a thin film deposited on a material (substrate)

The proportion of reflected and transmitted light is given by the reflection and transmission coefficients, which depend on the refractive index of the two media, the angle of incidence and the polarization of the light. The refractive index of ZnO is given, according to "refractive index", by the formula: [13-14].

$$n_{ZnO} = \sqrt{2.81418 + \left[\frac{0.87968.(\lambda.10^6)^2}{(\lambda.10^6)^2 - 0.3042^2} - 0.00711(\lambda.10^6)^2\right]} \quad (1)$$

And sapphire (Al2O3) by: [15-16]:

$$n_{Al_2O_3} = \sqrt{1 + \left[\frac{1.4313493(\lambda.10^6)^2}{(\lambda.10^6)^2 - 0.0726631^2} + \frac{0.65054713(\lambda.10^6)^2}{(\lambda.10^6)^2 - 0.1193242^2} + \frac{5.3414021(\lambda.10^6)^2}{(\lambda.10^6)^2 - 18.028251^2}\right]} \quad (2)$$

Reflection and transmission coefficients of ZnO in relation to air

Both reflection and transmission are governed by the Snell-Descartes laws.

At the interface between air ($n0$=1) and zinc oxide material with refractive index nZnO, the reflection in intensity under normal incidence is given by Fresnel's formulae:

$$R_{ZnO} = \left(\frac{n_0 - n_{ZnO}}{n_0 + n_{ZnO}}\right)^2 \quad (3)$$

As for the intensity transmission coefficient under normal incidence, its formula is given by:

$$T_{ZnO} = \frac{n_{ZnO}}{n_0} t_{ZnO}.t_{ZnO}^* \quad (4)$$

With

$$t_{ZnO} = \frac{2n_0}{n_0 + n_{ZnO}} \quad (5)$$

The refractive index depends on the wavelength of the incident light. Consequently, reflection and transmission coefficients are also wavelength-dependent. As a result, they vary with wavelength.

The absorption coefficient α of a material defines its capacity to absorb radiation (linearly). Its expression is given by the following relationship

$$\alpha = \frac{4\pi k}{\lambda} \quad (6)$$

With k the extinction coefficient corresponding to the absorption of the electromagnetic wave by the same material and λ the wavelength.

I-2 Reflection and transmission coefficients of sapphire (Al2O3) in relation to air

In the case of sapphire, its reflection coefficient under normal incidence with respect to air is:

$$R_{Al_2O_3} = \left(\frac{n_0 - n_{Al_2O_3}}{n_0 + n_{Al_2O_3}}\right)^2 \quad (7)$$

With $n0$ the index of air, which is equal to 1, and nAl_2O_3 the refractive index of sapphire (Al_2O_3).

And its transmission coefficient T in intensity under normal incidence; by the relation:

$$T = \frac{n_{Al_2O_3}}{n_0} t_{Al_2O_3} . t_{Al_2O_3}^{*} \quad (8)$$

With

$$t_{Al_2O_3} = \frac{2n_0}{n_0 + n_{Al_2O_3}} \quad (9)$$

I-3 Reflection and transmission coefficients of a layer-substrate stack: ZnO/sapphire

For a stack of ZnO/sapphire layers, instead of a matrix, we'll have a matrix product:

$$M = D_0 . C_1 . D_1 \quad (10)$$

With:

$$D_0 = \begin{pmatrix} \frac{n_0 + n_{ZnO}}{2n_0} & \frac{n_0 - n_{ZnO}}{2n_0} \\ \frac{n_0 - n_{ZnO}}{2n_0} & \frac{n_0 + n_{ZnO}}{2n_0} \end{pmatrix} \quad (11)$$

$$C_1 = \begin{pmatrix} e^{-i\Delta\varphi} & 0 \\ 0 & e^{+i\Delta\varphi} \end{pmatrix} \quad (12)$$

$$\Delta\varphi = \frac{2\pi n_{ZnO} e}{\lambda} \quad (13)$$

$$D_1 = \begin{pmatrix} \frac{n_{ZnO} + n_{Al_2O_3}}{2n_{ZnO}} & \frac{n_{ZnO} - n_{Al_2O_3}}{2n_{ZnO}} \\ \frac{n_{ZnO} - n_{Al_2O_3}}{2n_{ZnO}} & \frac{n_{ZnO} + n_{Al_2O_3}}{2n_{ZnO}} \end{pmatrix} \quad (14)$$

In this way, the reflection and transmission coefficients become:

$$r = \frac{M_{12}}{M_{22}} \quad (15)$$

$$R = r . r^{*} \quad (16)$$

$$t = \frac{1}{M_{22}} \quad (17)$$

$$T = \frac{n_{Al_2O_3}}{n_0} t . t^{*} \quad (18)$$

2. Results and Discussion

Figure 2 shows the evolution of the refractive index of ZnO and sapphire as a function of wavelength. Between 400 nm and 1000 nm, the refractive index of ZnO is almost linear. On the other hand, the refractive index of sapphire varies only slightly, decreasing in this wavelength range. ZnO is also found to be more refractive than sapphire.

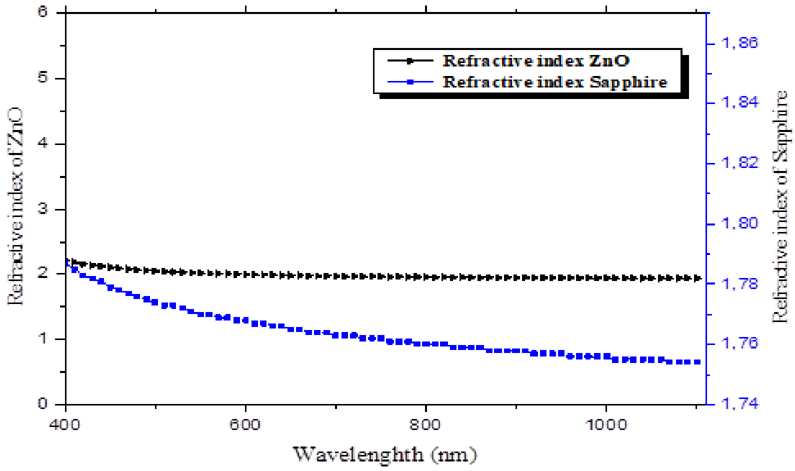

Figure 2: Variation in refractive index of ZnO and Sapphire as a function of wavelength

Figure 3 illustrates the optical reflection spectrum of zinc oxide (ZnO) over the wavelength range of 300 nm to 1000 nm. At 300 nm, the reflection coefficient exceeds 0.9 (90%), indicating that most incident light is reflected. This high reflection occurs because the energy of incoming photons is greater than ZnO's bandgap (3.3 eV), leading to absorption rather than transmission.

As the wavelength increases from 300 nm to 400 nm, a rapid decrease in reflection is observed, correlating with an increase in transmission. This shift indicates a reduction in ZnO's absorption capacity, as fewer photons possess sufficient energy to be absorbed. Consequently, more light is transmitted through the material.

In the visible and near-infrared regions (400 nm to 1000 nm), the transmission coefficient peaks at 0.89 (89%), demonstrating ZnO's transparency in this range. The high bandgap effectively prevents the absorption of lower-energy photons, making ZnO suitable for applications requiring high light transmission, such as LEDs and solar cells.

These optical properties underscore ZnO's versatility in optoelectronic applications, highlighting the importance of wavelength in determining its reflective and transmissive behaviors. Understanding these characteristics is essential for optimizing ZnO in future technologies.

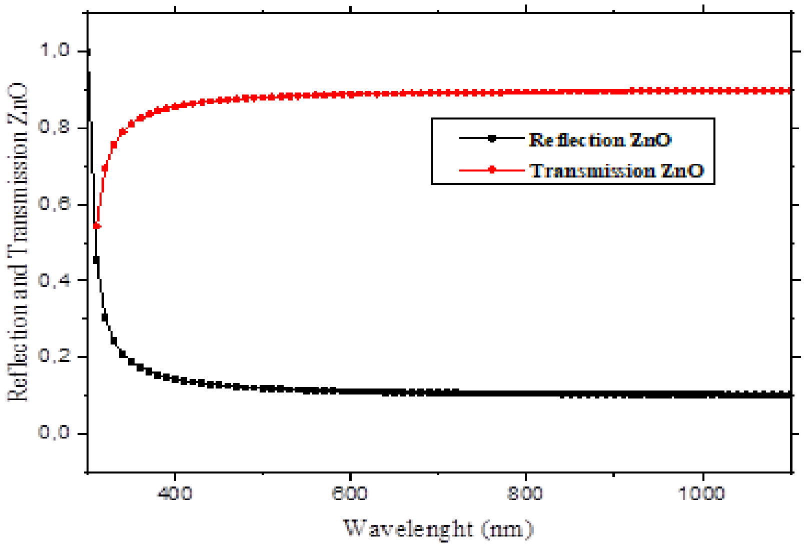

Figure 3: Variation in optical reflection and transmission of ZnO versus air as a function of wavelength

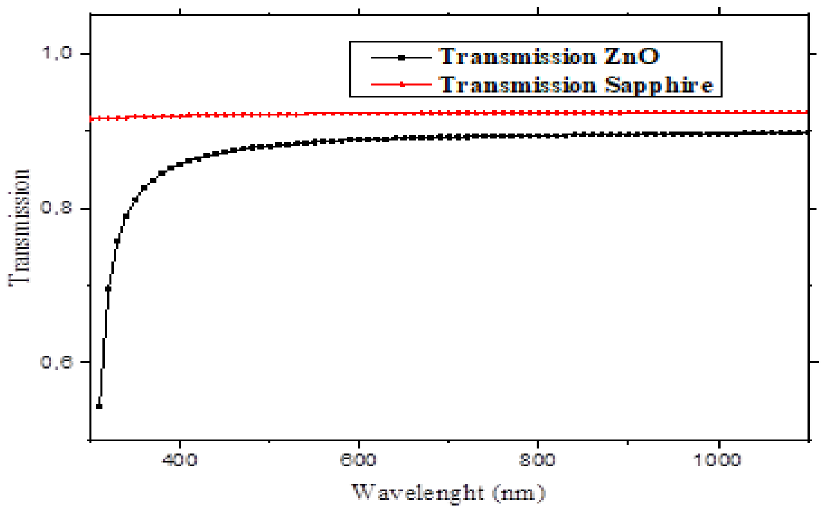

Figure 4: Variation of ZnO and sapphire transmission coefficients relative to air as a function of wavelength

Figure 4 clearly demonstrates that, across the entire studied wavelength range, the transmission coefficient of sapphire (Al_2O_3) consistently exceeds that of zinc oxide (ZnO). The maximum transmission observed for sapphire is 0.92 (92%), while that for ZnO peaks at 0.89 (89%). Notably, the transmission coefficient for sapphire appears nearly constant across the wavelengths measured, reflecting its stable optical properties. This observation is influenced by the scale used for both curves, which emphasizes the comparative performance of the two materials.

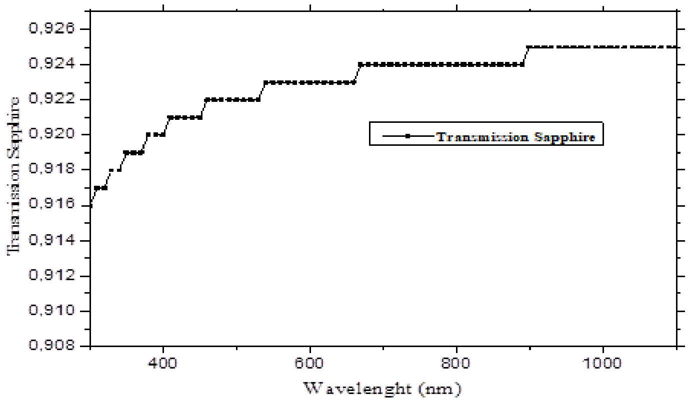

Figure 5: Variation in optical transmission of sapphire relative to air as a function of wavelength

However, a closer examination reveals that the transmission coefficient of sapphire does exhibit slight variations, ranging from 0.916 to 0.925, as illustrated in Figure 5. This subtle fluctuation can be attributed to the crystalline quality and surface finish of the sapphire, as well as potential scattering effects.

The superior transmission characteristics of sapphire are largely due to its wide bandgap of approximately 8.8 eV, which allows it to maintain high optical clarity across the visible, infrared, and ultraviolet regions. In contrast, ZnO is transparent only up to its bandgap of 3.3 eV, limiting its effective transmission to lower energy photons.

The high transmission of sapphire is also contingent on its surface quality; a well-polished surface enhances light transmission, while a rough or poorly polished surface can diminish it due to increased scattering and reflection. Given its excellent transmission properties, sapphire is ideally suited for applications in anti-reflective coatings, particularly when paired with materials like ZnO that require enhanced optical performance. This combination can significantly improve device efficiency in optical and optoelectronic applications.

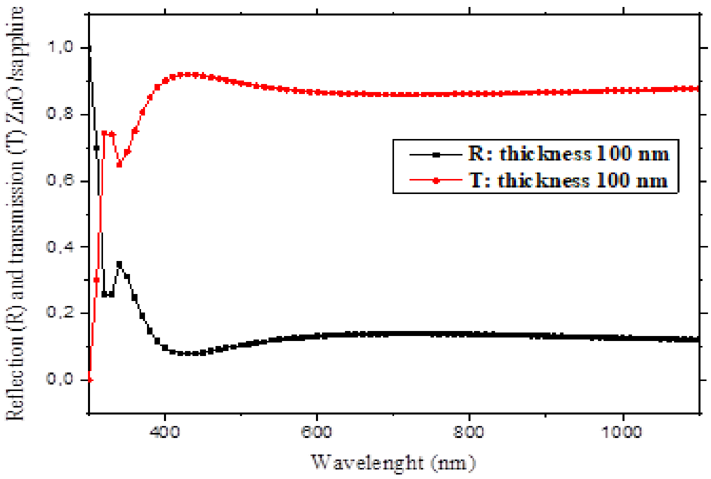

Figure 6: Evolution of the reflection and transmission coefficients of a ZnO layer deposited on Sapphire (Al_2O_3)

Figure 6 illustrates that within the wavelength range of 400 to 1000 nm, the optical transmission of zinc oxide (ZnO) reaches a maximum value of 0.92, concomitant with a minimum reflection coefficient of 0.08. This significant contrast underscores ZnO's effective transparency in this range, which is critical for various optoelectronic applications.

In contrast, wavelengths below 400 nm fall within the absorption region for ZnO. The absorption edge is observed between 365 and 385 nm [17], where a rapid decline in reflection occurs. This decline can be attributed to the absorption mechanisms associated with the electronic transitions between the valence band and the conduction band. In this spectral region, photons possess sufficient energy to excite electrons, leading to heightened absorption and consequently reduced reflection.

Moreover, the absorption of light at wavelengths greater than 400 nm is influenced by the presence of crystalline defects, including grain boundaries and dislocations [18]. These defects introduce localized energy states that can trap photons, contributing to the material's overall absorption characteristics. The interplay between these defects and the electronic band structure of ZnO is pivotal in understanding its optical behavior and optimizing its performance in practical applications.

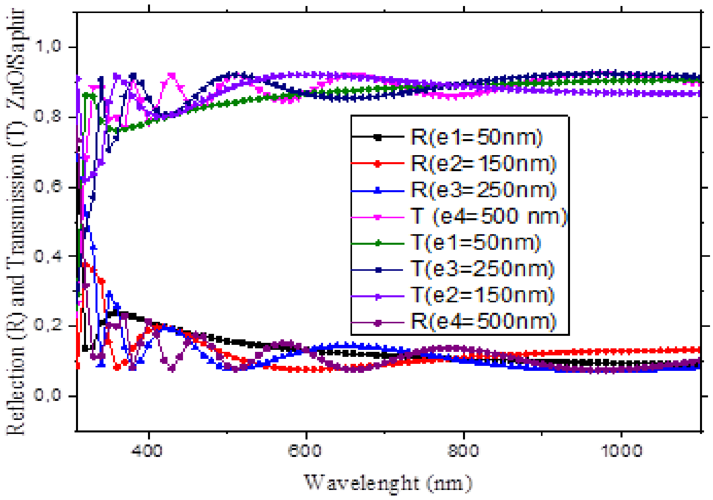

Figure 7: Reflection and optical transmission spectra of ZnO/sapphire with different thicknesses (e) as a function of wavelength (λ)

Figure 7 presents the optical reflection and transmission characteristics of zinc oxide (ZnO) films deposited on sapphire substrates, revealing that the number of interference maxima and minima increases with the thickness (e) of the ZnO layer. This phenomenon aligns with findings from N. Bouchenak Khelladi and N.E. Chabane Sari [19], who observed interference fringes within the wavelength range of 300 to 600 nm. For our study, transmission has maxima of about 0.92 and minima of about 0.60.

The enhanced optical transmission of the deposited films, relative to the maximum transmission of ZnO in air, can be attributed to the contributions from the sapphire substrate, whose transmission properties were characterized in Figure 4. The interference patterns arise from multiple reflections occurring between the lower surface in contact with the substrate and the upper free surface of the ZnO layer. This suggests that the ZnO may not uniformly cover the sapphire substrate following deposition, potentially due to lattice mismatch issues. Specifically, the lattice parameters of ZnO (a = 4.754 Å, c = 5.213 Å) differ significantly from those of sapphire (a = 4.754 Å, c = 12.99 Å), which can lead to defects and imperfections in the thin film.

In the wavelength range of 600 to 1000 nm, a slight decrease in transmission is noted, stabilizing around 0.88 across various film thicknesses. This range corresponds to a region of high transparency, indicating that while the films perform well optically, some absorption mechanisms may still be at play.

Our theoretical study further indicates that the maximum reflection values vary with film thickness, likely due to differences in surface roughness. Rougher films tend to scatter light more effectively, influenced by the nanoscale structures present on the film's surface [20]. Additionally, the degree of light scattering is wavelength-dependent, which can affect the overall optical performance of the ZnO films.

This analysis highlights the intricate interplay between film thickness, surface morphology, and substrate characteristics in determining the optical behavior of ZnO films on sapphire. Understanding these factors is crucial for optimizing ZnO for advanced optoelectronic applications.

3. Conclusion

The analyses conducted on the optical properties of zinc oxide (ZnO) antireflective coatings deposited on sapphire substrates reveal significant findings regarding optical transmission. Measurements indicate that the optical transmission of sapphire reaches a maximum value of 0.92, while ZnO achieves a transmission of 0.89 in the wavelength range of 400 to 1000 nm. Conversely, at 300 nm, the reflection of ZnO exceeds 90%, resulting in low transmission. The study also highlighted the presence of interference fringes within the 300 to 600 nm range, with transmission maxima at 0.92 and minima at 0.60. This indicates a strong influence of the ZnO layer's thickness; as thickness increases, the number of observed maxima and minima also increases, suggesting that the layer does not uniformly cover the substrate. This non-uniformity is likely due to lattice mismatch between ZnO and sapphire. Furthermore, between 600 and 1000 nm, transmission remains nearly constant at around 0.88. This stability indicates a region of high transparency, while the roughness of the film's surface may also affect light scattering. These results underscore the importance of utilizing a ZnO/sapphire antireflective coating to enhance optical performance. Optical transmission is influenced not only by the deposited material but also by the substrate's properties, particularly the refractive index and thickness. These elements are crucial for optimizing optoelectronic applications by maximizing light transmission efficiency.

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