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Contribution to the Study of the Electrical and Optical Properties of a Wide Band Gap Semiconductor

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ABSTRACT

In recent years, zinc oxide (ZnO) has attracted considerable attention as a promising semiconductor material owing to its natural abundance, low cost, and outstanding physical properties. With a wide and direct band gap of 3.3 eV at 300 K, high transparency in the visible region, and a large exciton binding energy of about 60 meV, ZnO has become a key material for a broad range of optoelectronic and photonic applications. In the present study, we examine the crystalline structure, as well as the electrical and optical properties of ZnO, focusing on doping mechanisms, characterization techniques, and their influence on material performance. Furthermore, structural, optical, and electrical investigations were carried out on thin ZnO films doped with 2 at.% aluminum (Al). The obtained results highlight the potential of Al-doped ZnO as an efficient transparent conductive oxide (TCO) for advanced electronic and optoelectronic devices.

Keywords : Zinc oxide (ZnO), Al-doping, thin films, structural and optical characterization, transparent conductive oxide (TCO).

Introduction

The field of materials science has undergone a profound transformation with the emergence of thin-film technology. The introduction of semiconductor materials into electronic components marked the first major technological milestone following the invention of the semiconductor transistor. As this technology matured, the electronics industry experienced exponential growth, enabling the fabrication of increasingly powerful, miniaturized, and cost-effective devices through large-scale manufacturing. The next technological leap came with the progressive integration of a greater number of electronic components within smaller volumes, thus initiating the continuous race toward device miniaturization. Materials with characteristic dimensions ranging from tens to hundreds of nanometers exhibit exceptional behaviors, as their physical properties differ markedly from those of

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their bulk counterparts [1]. Thin-film materials have found widespread use in modern technological applications such as light-emitting diodes (LEDs), laser devices, and photovoltaic cells [2–4].Among various semiconductor oxides, zinc oxide (ZnO) has emerged as a particularly promising material owing to its abundance, low cost, and superior physical properties [5–7]. Naturally occurring ZnO appears as a ruby-red mineral, while synthetically produced ZnO is typically white or colorless [8]. Its wide and direct band gap (3.37 eV) and large exciton binding energy (60 meV) at room temperature make it an ideal candidate for ultraviolet (UV) optoelectronic and photovoltaic applications [4]. When deposited as a thin film, ZnO can also serve as a transparent conductive electrode, a piezoelectric transducer, a gas sensor, or an optical waveguide material, owing to its high refractive index under optical excitation—an important feature in the design of guided-wave photonic systems [1].Given the growing scientific and technological interest in ZnO, the present work focuses on thin ZnO films doped with 2 at.% aluminum (Al). The objective is to contribute to the understanding of their structural, optical, and electrical properties for potential use in photovoltaic and optoelectronic applications [10–11].

Experimental Details

Objective

The main objective of the present work is to characterize the electrical and optical properties of a wide band gap semiconductor, namely zinc oxide (ZnO) doped with 2% aluminum (Al).

Substrate Preparation

The substrates used for the deposition of the studied material were obtained by cutting soda-lime glass slides using a Dicing-Cutting Saw, as illustrated in Figure .1 below.

Substrate Cleaning Procedure

Prior to the deposition of ZnO-based thin films, the glass substrates were thoroughly cleaned according to the following procedure:

- Cleaning with a detergent in an ultrasonic bath;
- Rinsing with deionized (DI) water;
- Cleaning with acetone in an ultrasonic bath;
- Cleaning with isopropyl alcohol (IPA) in an ultrasonic bath;
- Rinsing with DI water;
- Drying under a nitrogen (N_2) flow.

This multi-step cleaning ensures the removal of organic and particulate contaminants, providing a smooth and clean surface for thin-film deposition.

Deposition of ZnO:Al (2%) Thin Films

The ZnO thin films doped with 2% Al were deposited using a cathodic sputtering system, as shown in Figure.2.

The experimental conditions for the deposition process were as follows:

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- Base pressure: **4 × 10^{-7} mbar**
- Working pressure: **2.5 × 10^{-6} mbar**
- Power: **90 W**
- Deposition rate: **1 Å/s**
- Film thickness: **150 nm**
- Target material: **ZnO doped with 2% Al** (purity: **99.99%**)

These parameters were optimized to obtain uniform and adherent thin films with good structural and optical quality.

Contact Deposition

Electrical contacts were deposited using an electron-beam evaporation system (Minilab 60, Moorfield) under the following experimental conditions:

- Base pressure: **2.6 × 10^{-7} mbar**
- Working pressure: **3.2 × 10^{-6} mbar**
- Power: **110 W**
- Deposition rate: **1 Å/s**
- Film thickness: **250 nm**
- Contact material: **Silver (Ag)** (purity: **99.99%**)

This technique ensures highly conductive and well-adhered contacts suitable for electrical characterization of the thin films.

Physicochemical Characterization

After the deposition of the thin film, the phase composition of the deposited layer was analyzed using an Equinox 3000 X-ray diffractometer (Figure.3).The diffraction pattern revealed a prominent (002) peak appearing at approximately 34° (Figure .4), which confirms the formation of ZnO with a preferential growth along the c-axis of its hexagonal wurtzite structure. This indicates a well-oriented crystalline film with typical ZnO phase characteristics.

Optical Characterization

The transmittance **and** reflectance spectra of the deposited films were recorded using an F10-RT-UV spectrophotometer**,** as shown in Figure .5**.**

Transmittance Spectrum

Figure.6 presents the **transmittance spectrum** of ZnO/2%Al thin films. The transmittance in the **visible region** exceeds **75%**, indicating high optical transparency, whereas a strong absorption is observed **below 300 nm**, which is attributed to both the **glass substrate** and the **ZnO:Al layer**. The **absence of interference fringes** in the visible range suggests that the deposited film is **very thin (approximately 150 nm)**, consistent with the deposition parameters.

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Reflectance Spectrum

Figure.7 shows the reflectance spectrum of the ZnO/2%Al thin films. The reflectance is found to be very low in the UV region and remains below 10% in the visible range, confirming the high transparency and optical quality of the deposited layer.

Optical Properties and Band Gap Determination

The high transmittance and low reflectance of the Al-doped ZnO thin films make this material a promising candidate for use as a transparent electrode or as an antireflection coating in solar cell applications.

Optical Band Gap Determination

The optical absorption coefficient (α) in the fundamental absorption region was determined for various photon energies from the transmission spectra using the following relation:

$$\alpha = -\ln(T)/d$$

where d is the film thickness and T is the transmittance.

The optical band gap of the films was determined by applying the Tauc and Davis–Mott models in the high-absorption region using the following expression:

$$\alpha h\nu = A(h\nu - E_g)^n$$

where α is the absorption coefficient, hν is the photon energy, Eg is the optical band gap, and A is a constant.

For n = 1/2, the transition data provided the best linear fit in the band-edge region, indicating a direct allowed transition. The band gap of the films can be deduced from the plot of $(\alpha h\nu)^2$ as a function of photon energy hν by extrapolating the linear portion of this plot (expression 3) to the energy axis, as shown in Figure.8. The estimated optical band gap was found to be 3.85 eV.

Electrical Characterization

The structure prepared for electrical characterization consists of a ZnO/2%Al-based thin film with a thickness of 150 nm deposited on a glass substrate, with four silver contacts of 250 nm thickness deposited at the corners of the structure (Figure IV.8). The electrical measurements carried out at room temperature using the four-point probe (Figure IV.10) and the Hall effect system (Figure IV.11) are summarized in Tables IV.1 and IV.2, respectively. The resistivities obtained from both instruments are of the same order of magnitude, indicating that the doped ZnO oxide is conductive. because the measured resistivity is within the range typical of doped semiconductors (on the order of 20 Ω·cm).

Discussion and Interpretation

The intrinsic properties of zinc oxide (ZnO)—including its crystallographic structure and electronic band configuration—make it a highly versatile and technologically significant material, suitable for various applications.

In this study, we investigated Al-doped ZnO thin films (2% Al) deposited using a cathodic sputtering system. The electrical contacts were fabricated by electron-beam evaporation (Minilab 60, Moorfield).

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To obtain comprehensive information about the prepared samples, several characterization techniques were employed:

- Structural characterization was carried out using an Equinox 3000 X-ray diffractometer to identify the crystalline phases.
- Optical characterization was performed using an F10-RT-UV spectrophotometer to analyze the transmittance and reflectance spectra.
- Electrical characterization was conducted on the ZnO:Al thin films deposited on glass substrates with four silver electrodes positioned at the corners of the structure to assess conductivity and resistivity.

These combined analyses provide a detailed understanding of the structural, optical, and electrical behaviors of Al-doped ZnO thin films, confirming their potential for transparent conductive oxide (TCO) and photovoltaic device applications.

The structural characterization of the deposited films allowed the identification of the crystalline phases using an X-ray diffractometer, which revealed a pronounced (002) diffraction peak around 34°, confirming the formation of ZnO with a preferred growth orientation along the c-axis of the wurtzite crystal structure.

The optical characterization provided the reflectance and transmittance spectra, from which the following observations were made:

- The transmittance in the visible region exceeds 75%, while a strong absorption occurs below 300 nm, attributed to both the glass substrate and the ZnO:Al (2%) layer. The absence of interference fringes in the visible region indicates that the deposited film is very thin (approximately 150 nm).
- The reflectance is negligible in the UV region and remains below 10% in the visible range.

These results demonstrate that the high transmittance and low reflectance of the Al-doped ZnO (2%) films make this material a promising candidate for use as a transparent electrode or as an antireflection coating in solar cell applications.

The transmission spectra were also used to determine the optical absorption coefficient (α) in the fundamental absorption region for different photon energies. The optical band gap (Eg) of the films was calculated by applying the Tauc and Davis–Mott models in the high-absorbance region. The obtained results indicate that the optical band gap is approximately 3.85 eV, which is consistent with typical values for Al-doped ZnO thin films.

Finally, regarding the electrical characterization, the prepared structure consisted of a ZnO:Al (2%) thin film with a thickness of 150 nm, deposited on a glass substrate and equipped with four silver contacts (each 250 nm thick) positioned at the corners of the sample. Electrical measurements performed at room temperature using both a four-point probe and a Hall effect measurement system revealed resistivity values of the same order of magnitude. The results confirm that the Al-doped ZnO film exhibits semiconducting conductivity, with a measured resistivity on the order of 20 Ω·cm, typical of doped semiconductor materials.

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Figures

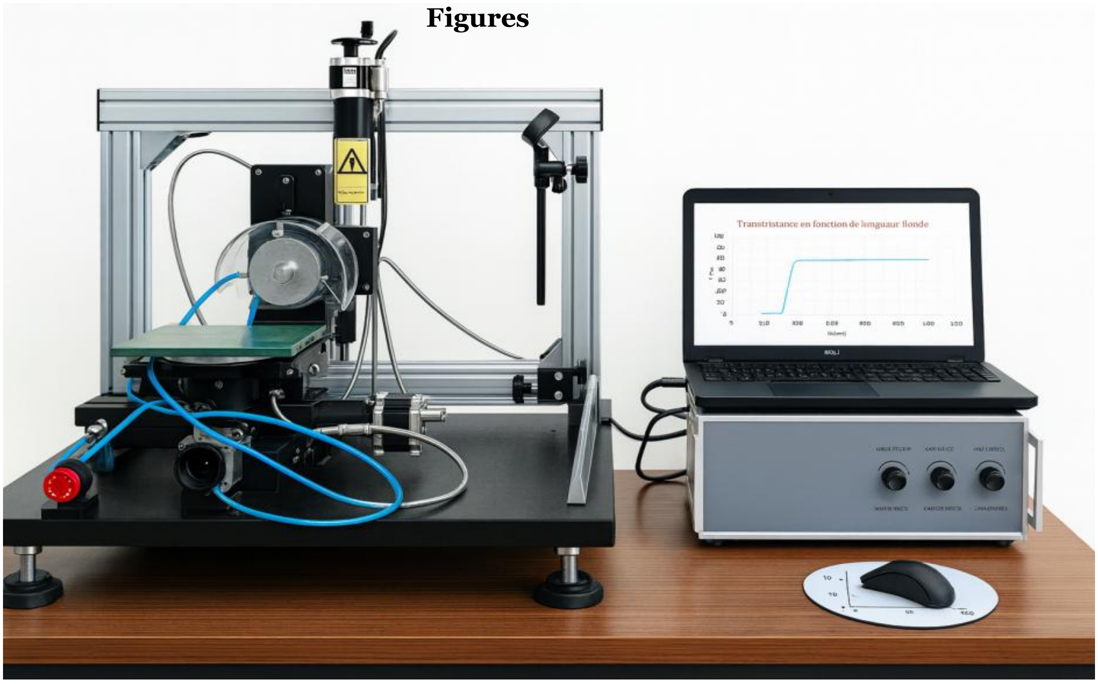

Figure1: Substrate cutting machine, Clean Room

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Figure 2 : The sputtering system, Clean Room

Figure 3 :Equinox 3000 diffractometer used to determine the phases

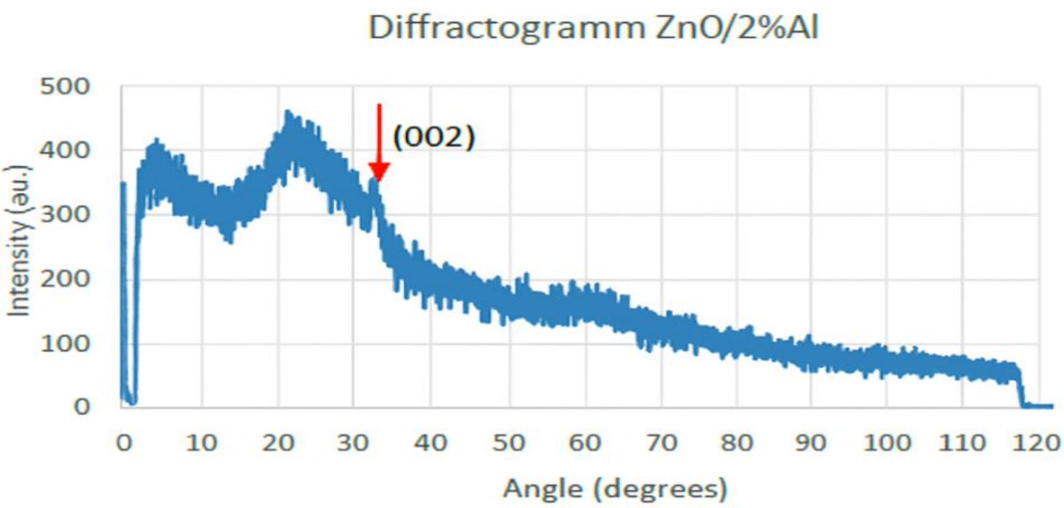

Figure 4 : Diffractogram of ZnO/2%Al

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Figure 5 : F10-RT-UV spectrometer used for optical measurements

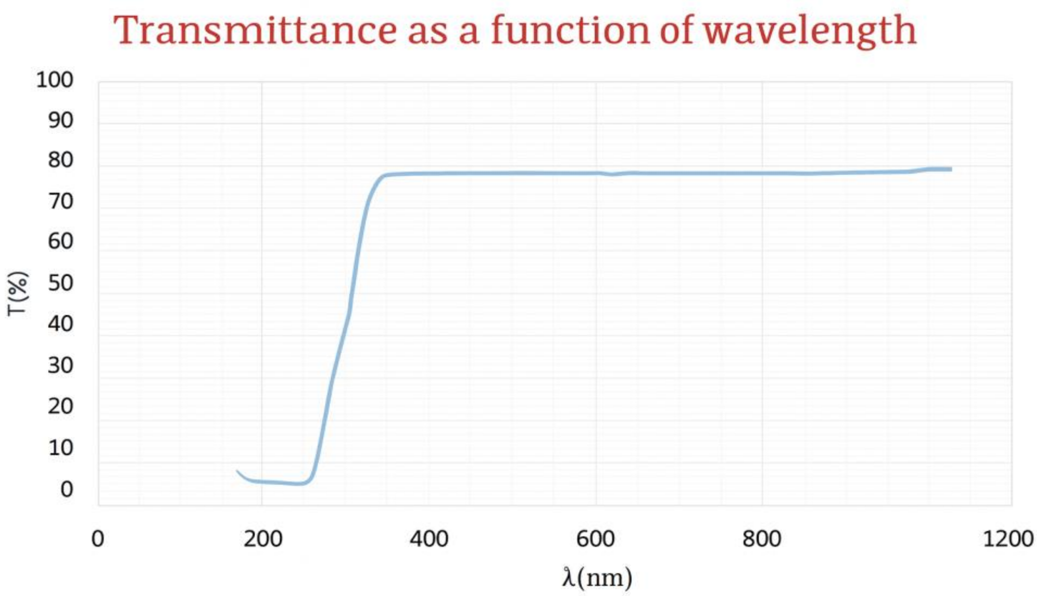

Figure 6 : Transmittance spectrum of ZnO/2%Al layers

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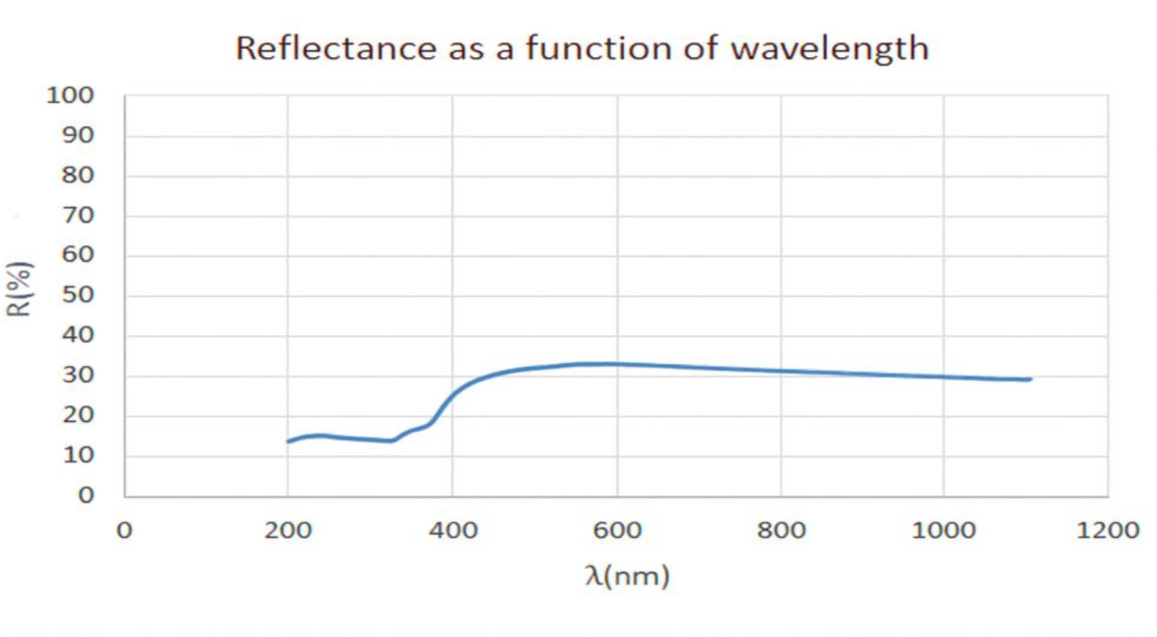

figure 7 : Reflectance spectrum of ZnO/2%Al layers

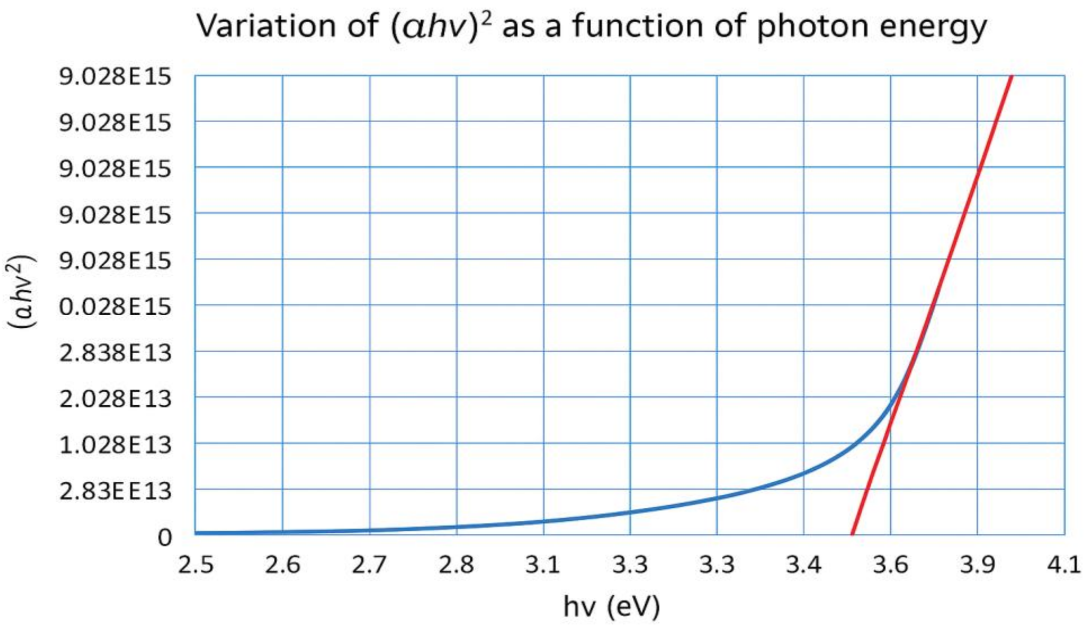

Figure 8 : Variation of $(\alpha h\nu)^2$ as a function of photon energy

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Tableaux

N°	T(K)	ρ (Ω)	Vmes aux bornes Rstand (mV)	Vmes (mV)	Range I (μA)
01	297	28.51	99.00	415.2	1
02	297	20.36	99.11	269.9	1
03	297	19.85	99.08	289.IV	1
04	297	19.88	99.01V	289.6	1

Tableau1:Electrical measurements obtained using the four-point probe

N	T(K)	I(A)	ρ (Ω.cm)
1	297	-5,00E-09	21.90
2	297	-4,00E-09	21.60
3	297	-3,00E-09	21.00
4	297	-2,00E-09	20.00
5	297	-1,00E	17.50
6	297	2,07E-25	19.30
7	297	1,00E-09	1,61E+01
8	297	2,00E-09	1,99E+01
10	297	3,00E-09	2,04E+01

Tableau 2:Electrical measurements obtained using the Hall effect system