"Investigation of Structural and Optical Properties of Synthesized ZnO Thin Films"

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Abstract

Pure zinc oxide (ZnO) thin films were successfully synthesized using a chemical deposition technique on glass substrates to investigate their structural and optical properties. The structural characteristics of the films were examined by X-ray diffraction (XRD), which confirmed the formation of a single-phase hexagonal wurtzite ZnO structure with good crystallinity and a preferred orientation along the (002) plane. The calculated lattice parameters were found to be in close agreement with standard ZnO values, indicating low structural distortion and high phase purity. Microstructural parameters such as crystallite size, lattice strain, and dislocation density revealed that the films possess uniform grain growth and minimal defect concentration. Optical properties were studied using UV–Visible spectroscopy in the wavelength range of 300–800 nm. The ZnO thin films exhibited high optical transparency in the visible region with a sharp absorption edge in the ultraviolet region. The optical band gap was estimated using Tauc's plot, assuming a direct allowed transition, and was found to be approximately 3.27 eV. The observed band gap value is consistent with bulk ZnO and suggests good optical quality of the deposited films. The combination of high crystallinity, wide band gap, and optical transparency makes pure ZnO thin films promising candidates for applications in optoelectronic devices, transparent electrodes, and gas sensing applications.

Keywords: - Pure ZnO thin films, Structural properties, Optical properties, X-ray diffraction (XRD), UV–Visible spectroscopy, Optical band gap, Wurtzite structure

1. Introduction

Zinc oxide (ZnO) is a widely studied II–VI semiconductor owing to its excellent structural, optical, and electrical properties. It possesses a wide direct band gap of ~3.3 eV at room temperature along with a large exciton binding energy of about 60 meV, which enables efficient excitonic emission even at ambient conditions [1,2]. These unique features make ZnO an attractive material for diverse applications such as ultraviolet light-emitting diodes, photodetectors, transparent conducting oxides, gas sensors, solar cells, and piezoelectric devices [3–5]. In addition, ZnO is chemically stable, non-toxic, earth-abundant, and cost-effective, which further supports its extensive use in modern optoelectronic technologies.

Structurally, ZnO crystallizes predominantly in the hexagonal wurtzite phase under normal conditions, belonging to the space group $P6_3mc$ [6]. In this structure, each Zn^{2+} ion is tetrahedrally coordinated with four O^{2-} ions, resulting in strong ionic–covalent bonding. The non-centrosymmetric nature of the wurtzite lattice along the c-axis gives rise to spontaneous polarization, piezoelectricity, and pyroelectricity [7]. The structural quality of ZnO thin films—such as crystallite size, preferred orientation, lattice strain, and defect density—significantly influences their optical absorption, transparency, and charge transport properties. Therefore, understanding the relationship between structure and optical behavior is essential for improving device performance [8].

ZnO thin films can be fabricated using several deposition techniques, including radio-frequency sputtering, pulsed laser deposition, chemical vapor deposition, sol–gel spin coating, and spray pyrolysis [9–11]. Among these, chemical deposition methods are particularly attractive due to their simplicity, low processing cost, scalability, and suitability for large-area coatings. These methods also allow control over microstructural properties by tuning deposition parameters such as temperature, precursor concentration, and annealing conditions [12].

Optical characterization of ZnO thin films provides critical insight into their electronic band structure and defect states. UV–Visible absorption spectroscopy is commonly used to evaluate optical transparency and absorption edge behavior. The optical band gap is generally estimated using Tauc's relation for direct allowed transitions [13]. Variations in band gap values are often attributed to crystallinity, strain, grain size effects, and intrinsic defects such as oxygen vacancies and zinc interstitials [14].

In this work, pure ZnO thin films are synthesized using a chemical deposition technique, and their structural and optical properties are systematically investigated using X-ray diffraction and UV–Visible spectroscopy. The study aims to correlate microstructural characteristics with optical band gap behavior to assess the suitability of pure ZnO thin films for optoelectronic and sensing applications.

2. Materials and Methods

2.1 Materials

Analytical reagent (AR) grade zinc acetate dihydrate was used as the precursor material without further purification. Distilled water served as the solvent for solution preparation. Microscope glass slides were employed as substrates due to their smooth surface, thermal stability, and suitability for optical characterization of ZnO thin films.

2.2 Precursor Preparation

The precursor solution was prepared by dissolving an appropriate amount of zinc acetate dihydrate in distilled water to obtain the desired molarity. The solution was magnetically stirred at room temperature until complete dissolution, resulting in a clear and homogeneous solution suitable for spray pyrolysis deposition.

2.3 Substrate Cleaning

Glass substrates were thoroughly cleaned to remove surface contaminants. They were sequentially washed with detergent, distilled water, acetone, and ethanol, followed by ultrasonic cleaning. The substrates were finally dried in air to ensure a clean and uniform surface for film deposition.

2.4 Spray Pyrolysis Technique

ZnO thin films were deposited using a spray pyrolysis setup, as shown in Fig. 1. The prepared precursor solution was atomized and uniformly sprayed onto thoroughly cleaned glass substrates that were preheated to an optimized deposition temperature. During the spraying process, fine droplets of the solution reached the hot substrate surface, where they underwent rapid solvent evaporation followed by thermal decomposition of the precursor. This process led to the formation of a continuous and adherent ZnO thin film. The substrate temperature played a crucial role in controlling the decomposition rate and film quality. As shown in Fig. 2, the deposited films exhibited uniform surface coverage, good adhesion to the glass substrate, and suitable mechanical stability, showing the effectiveness of the spray pyrolysis technique for ZnO thin film preparation.

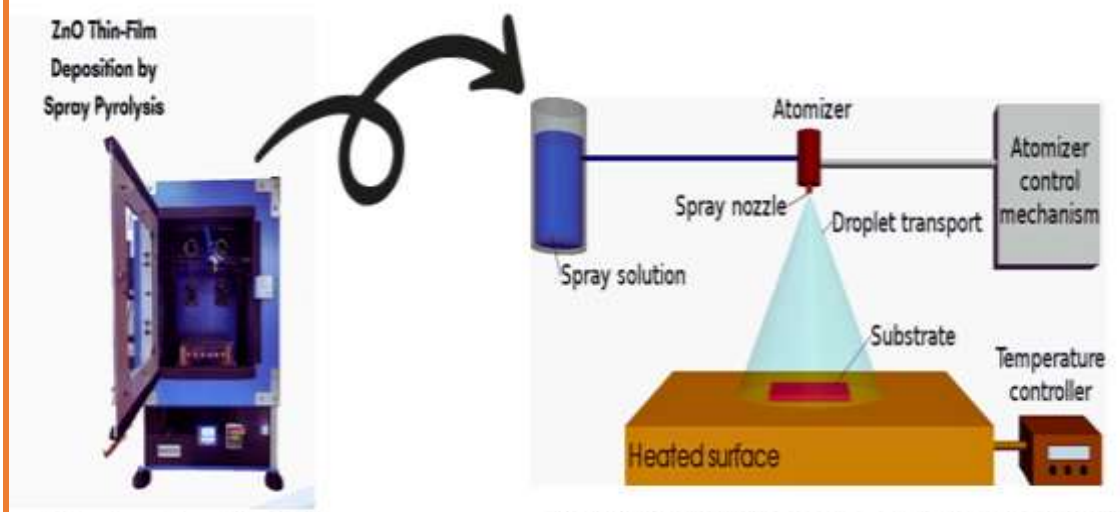

Fig. 1:- Spray Deposition Machine

Fig. 2:- Spray deposition process on pre-heated glass substrate at 400°C Temperature

Figure 1 & Figure 2: Spray pyrolysis deposition setup and formation of uniform ZnO thin film on preheated glass substrate.

2.5 Characterization Techniques

The structural properties of the ZnO thin films were studied using X-ray diffraction (XRD). Optical properties were analyzed by UV–Visible spectroscopy to determine transparency and band gap. Microstructural parameters such as crystallite size, strain, and dislocation density were evaluated from XRD data.

3. Results and Discussion

3.1 XRD Pattern of ZnO Thin Film

Figure 3 shows the X-ray diffraction (XRD) pattern of the pure ZnO thin film. The diffraction pattern confirms the formation of a single-phase hexagonal wurtzite structure without any secondary or impurity phases. All observed peaks match well with the standard JCPDS data for ZnO, indicating high phase purity. The presence of a strong and sharp (002) diffraction peak suggests a preferred c-axis orientation perpendicular to the substrate surface, reflecting good crystalline quality of the deposited film. The average crystallite size was calculated using the Scherrer formula, while lattice strain and dislocation density were estimated from the broadening of the diffraction peaks, providing insight into the microstructural characteristics of the ZnO thin film.

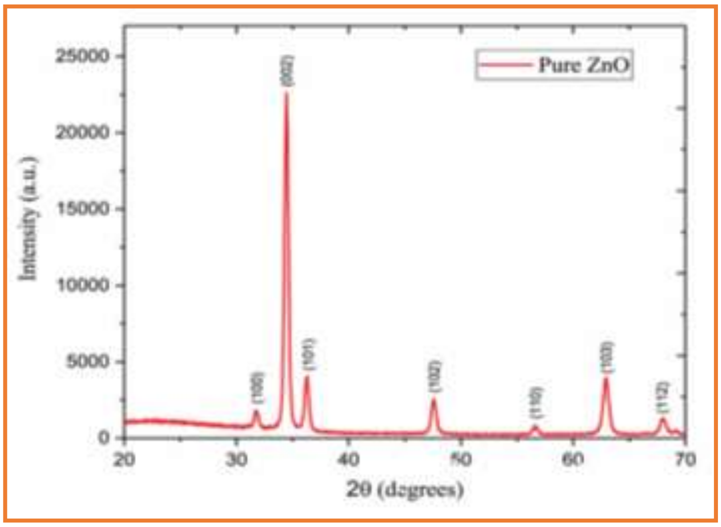

Figure 3: X-ray diffraction (XRD) pattern of pure ZnO thin film deposited on glass substrate

Table 1. Structural Parameters of Fe-Doped ZnO Thin Films

Sample	FWHM (rad)	a = b (Å)	c (Å)	c/a	Crystallite Size D (nm)	Dislocation Density ($\times 10^{15}$ lines/m²)	Lattice Strain (ε)	Unit Cell Volume e (Å³)	Bond Length (Å)	Atomic Packing Fraction (APF)
Pure ZnO	0.00737	3.2496	5.2018	1.6007	21.02	2.30	0.001658	47.57	1.9771	0.7550

The calculated lattice parameters closely match standard ZnO values, indicating minimal lattice distortion. These results demonstrate that the spray pyrolysis technique produces structurally well-defined ZnO thin films suitable for optoelectronic applications.

3.2 UV–Visible Spectroscopy

The optical properties of the ZnO thin film were investigated using UV–Visible spectroscopy in the wavelength range of 300–800 nm. The film exhibits high transparency in the visible region with a sharp absorption edge in the ultraviolet region, characteristic of ZnO. The optical band gap was determined using Tauc's plot by assuming a direct allowed transition. The estimated band gap value of approximately 3.27 eV is consistent with reported values for pure ZnO thin films. The sharp absorption edge indicates good crystallinity and low defect concentration. These optical characteristics make the ZnO thin film promising for transparent optoelectronic and sensing applications.

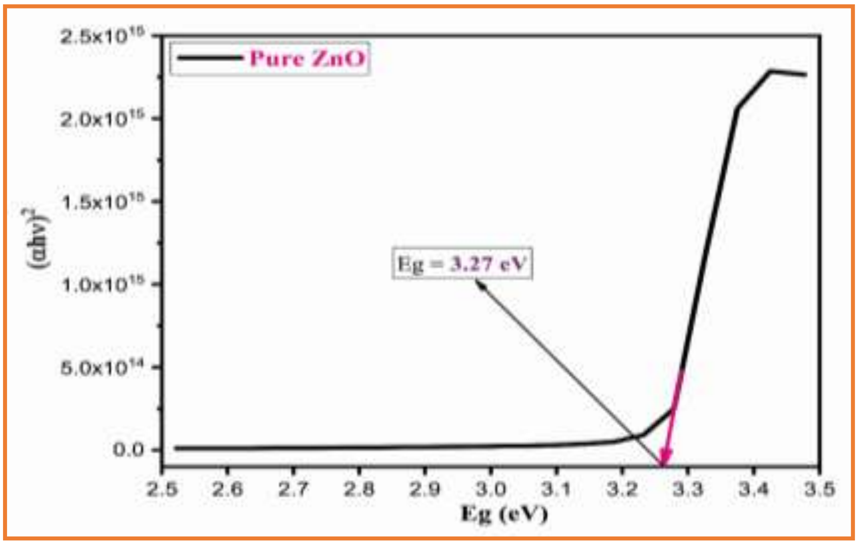

Figure 4: Tauc plot of pure ZnO thin film showing optical band gap (Eg = 3.27 eV)

4. Conclusions

Pure ZnO thin films were successfully synthesized using the spray pyrolysis technique, and their structural and optical properties were systematically investigated. X-ray diffraction analysis confirmed the formation of a single-phase hexagonal wurtzite structure with good crystallinity and a preferred c-axis orientation. The absence of secondary phases indicates high purity of the deposited films. Microstructural parameters such as crystallite size, lattice strain, and dislocation density revealed uniform grain growth with low defect concentration. UV–Visible spectroscopy showed high optical transparency in the visible region along with a sharp absorption edge in the ultraviolet region. The optical band gap was estimated to be approximately 3.27 eV, which is in good agreement with reported values for pure ZnO. The combined structural and optical results demonstrate that the prepared ZnO thin films possess desirable qualities for optoelectronic applications. Owing to their wide band gap, good crystallinity, and optical transparency, these films are suitable candidates for applications in transparent electrodes, ultraviolet photodetectors, and gas sensing devices.

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