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THE RELATIONSHIP BETWEEN STRUCTURAL DEFECTS AND ELECTRICAL CONDUCTIVITY IN ZnO THIN FILMS: AN INTERDISCIPLINARY RESEARCH APPROACH

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Abstract. This paper discusses the relationship between structural defects and electrical conductivity in zinc oxide (ZnO) thin films from an interdisciplinary perspective. The possible roles of oxygen and zinc vacancies, interstitial atoms, grain boundaries and lattice disorder in determining carrier concentration and mobility are reviewed. Combining X-ray diffraction, photoluminescence, Hall-effect and four-point-probe measurements is proposed as a practical strategy for connecting structural information with electrical properties. All figures and conceptual curves in this manuscript are schematic illustrations rather than measured experimental data.

Keywords: ZnO, thin films, structural defects, oxygen vacancy, grain boundaries, electrical conductivity, XRD, Hall effect.

Introduction. Zinc oxide (ZnO) is a II–VI semiconductor characterized by a direct band gap of approximately 3.3–3.4 eV at room temperature and a significant exciton binding energy. Consequently, it is considered a promising material for applications such as ultraviolet photodetectors, transparent conductive layers, gas sensors, p–n and heterojunction structures, and solar energy devices [1–3]. However, device efficiency depends not only on chemical composition but also on crystal quality, grain size, the type of defects present, and their spatial distribution.

The formation of defects in thin films is influenced by the synthesis method, precursor composition, chemical potential of oxygen, substrate temperature, annealing regime, and film thickness. Techniques such as sol-gel, spin-coating, spray pyrolysis, and magnetron sputtering can result in varying grain structures, textures, and defect concentrations. Therefore, it is essential to conduct structural analysis in conjunction with electrical measurements. The primary objective is to synthesize the physical relationships between the main defects in ZnO thin films and their electrical conductivity, as well as to propose an interdisciplinary research framework that integrates structural, optical, and electrical diagnostic methods.

Under ambient conditions, ZnO crystallizes in a hexagonal wurtzite crystal structure. Each Zn atom is tetrahedrally coordinated with four O atoms, and each O atom is tetrahedrally coordinated with four Zn atoms. In an ideal crystal, atoms are arranged in a periodic lattice; however, in actual thin films, point defects, dislocations, grain boundaries, and surface states may be present.

A vacancy is the absence of an atom from its regular position in a crystal lattice. An oxygen vacancy (V_o) refers to the absence of an oxygen atom from its lattice site, while a zinc vacancy (VZn) is an empty space at a zinc site. An interstitial atom (for example, Zni) occupies a position between the regular lattice sites. Additionally, foreign atoms may occupy positions normally held by zinc or oxygen. Whether a defect is electrically active or passive depends on its charge state, its formation energy, and the Fermi level.

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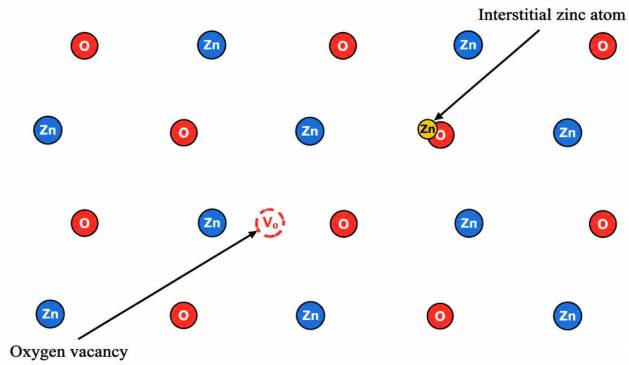


Figure 1. Schematic representation of defects in the ZnO crystal lattice. V_o — oxygen vacancy; Zn_i — interstitial zinc atom. The figure is provided for illustrative purposes.

An important caveat is that oxygen vacancies cannot be considered the sole—or even consistently effective—source of n-type conductivity in ZnO. Theoretical and experimental studies indicate that certain defects can create deep-level states, act as compensating centers, or influence optical signals. To accurately identify the sources of charge carriers, one must collectively account for defect chemistry, impurities, surface adsorption, and experimental conditions [2,3].

METHODS AND ANALYSIS. This study investigates the relationship between structural defects and electrical conductivity in ZnO (zinc oxide) thin films. The research methodology integrates theoretical foundations from solid-state physics, crystallography, materials science, and semiconductor electronics. The primary focus is on analyzing how defects within the crystal lattice affect charge carrier concentration, mobility, and the resulting electrical conductivity.

Structural defects in ZnO thin films can form depending on synthesis conditions, annealing temperature, oxygen content, film thickness, and the degree of crystallinity. Such defects include oxygen vacancies, zinc vacancies, interstitial atoms, dislocations within the crystal lattice, and defect states at grain boundaries. A comprehensive approach—utilizing structural, optical, and electrical diagnostic methods—is essential for evaluating their physical properties.

X-ray diffraction (XRD) can be employed to study the crystal structure and structural parameters of ZnO thin films. Based on the position, intensity, and full width at half maximum (FWHM) of diffraction peaks, XRD analysis enables the assessment of the crystalline phase, crystallization characteristics, and microstructural variations. Under ambient conditions, ZnO possesses a hexagonal wurtzite crystal structure. The characteristic peaks observed in the diffractogram confirm the presence of this crystalline phase. While peak broadening may be related to crystallite size and microstrain, instrumental broadening must also be taken into account.

Electrical resistance can be evaluated using the four-probe method, while charge carrier concentration and mobility can be assessed via the Hall effect. Applying these methods in combination helps determine whether changes in electrical conductivity are linked to carrier concentration or carrier mobility. In ZnO thin films, structural defects influence electrical conductivity through various mechanisms. Some defects may donate or accept electrons, while others act as charge-carrier trapping centers or scattering centers. Consequently, variations in electrical conductivity depend on the type of defects, their charge state, and their distribution within the crystal lattice [4].

When evaluating the impact of oxygen vacancies, it is necessary to consider their electrically active states, the conditions under which they form, and their interactions with other defects. Oxygen

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vacancies cannot be assumed to be the sole source of free electrons in all ZnO films. Electrical properties may also be influenced by foreign impurities, surface adsorption, compensating defects, and grain boundaries.

Defects at grain boundaries can trap charges and create potential barriers. This phenomenon is likely to reduce electron mobility and increase the overall resistance of the film. On the other hand, an increase in the concentration of electrically active donors can raise the number of free electrons, potentially leading to higher electrical conductivity. Consequently, the relationship between the density of structural defects and electrical conductivity is not always monotonic. To reliably assess this relationship, XRD results should be compared with electrical measurements, photoluminescence spectra, and—where available—data on the chemical composition of the surface.

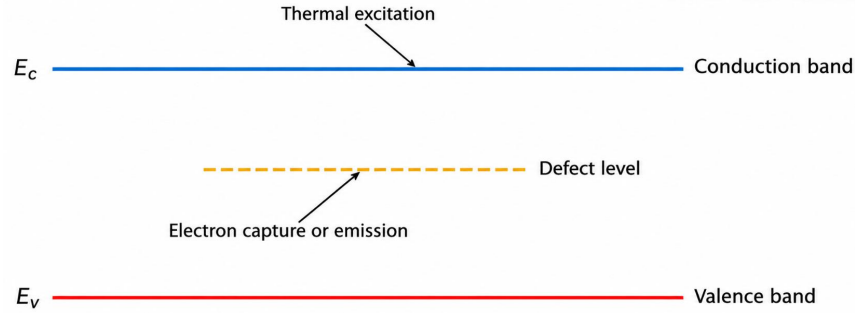


Figure 2. A simplified diagram showing the emergence of a defect level within the energy gap. This is a conceptual illustration and does not provide specific defect energy values.

When comparing ZnO thin films annealed at different temperatures, other technological parameters must be kept as consistent as possible. For instance, XRD and electrical measurements for samples processed at 300 °C, 400 °C, and 500 °C should be conducted using the same methodology. In this process, it is crucial to isolate the effect of temperature from variations in film thickness, contact resistance, and measurement conditions.

Electrical conductivity, σ, is determined by the charge carrier concentration, n (or hole concentration, p), the elementary charge, q, and the mobility, μ. In cases where electrons are the dominant carriers, a simplified expression can be written as $\sigma=qn\mu$. Defects can alter n - for instance, by trapping electrons - or they can reduce μ by acting as scattering centers. Consequently, an increase in the number of defects does not necessarily lead to an increase in electrical conductivity. Grain boundaries can create charge-trapping states and potential barriers; as a result, electrons moving between grains may undergo additional scattering or encounter barriers that they must overcome. On the other hand, certain defects can function as donors, thereby increasing the concentration of free electrons. The resulting electrical property is determined by the combined effect of these competing mechanisms [5].

The simplified expression for the electrical conductivity of a homogeneous layer is as follows:

$$\sigma = q(n\mu_n + p\mu_p)$$

Here, q is the elementary charge, n and p are the concentrations of electrons and holes, respectively, and μ_n and μ_p are their respective mobilities. If electrons are the majority charge carriers in the layer, it can be assumed that $\sigma \approx qn\mu_n$. The resistivity is given by $\rho = 1/\sigma$. In the four-probe method, the resistance or resistivity is determined by taking into account the geometry and thickness of the layer;

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meanwhile, Hall measurements help in evaluating the type, concentration, and mobility of the charge carriers.

RESULTS. X-ray diffraction (XRD) is an important technique for analyzing the structural properties of ZnO thin films. This method allows for the assessment of the crystalline phase, the degree of order within the crystal lattice, the width of the diffraction peaks, and the average crystallite size. ZnO typically crystallizes in a hexagonal wurtzite crystal structure. However, the crystalline quality of the layer may depend on the deposition method, the thermal treatment temperature, the layer thickness, and the properties of the substrate material. If a decrease in the width of diffraction peaks is observed following thermal treatment, this may be attributed to an increase in crystallite size or a reduction in microstrain within the crystal lattice. However, when drawing this conclusion, it is necessary to distinguish between these two factors and also account for instrumental broadening.

The impact of defects depends on their type, charge state, energy level, and position within the crystal lattice. Some defects can facilitate the generation of charge carriers or alter their concentration. Others may act as electron-trapping centers, thereby reducing the number of free charge carriers. Furthermore, grain boundaries and structural disorders can enhance electron scattering, potentially lowering electron mobility.

It is inaccurate to view oxygen vacancies as the sole or consistently effective source of donors influencing the electrical conductivity of ZnO. The electrical activity of defects is determined by their physicochemical nature; for instance, certain vacancies may create deep energy levels. Consequently, additional experimental evidence is required before attributing any increase or decrease in electrical conductivity to a single type of defect.

Thermal treatment of ZnO thin films can influence the crystallization process, crystallite size, residual stresses, and the state of defects within the film. Under certain conditions, an increase in temperature promotes crystal growth and improves the ordering of the crystal lattice. At the same time, the atmosphere, duration, and cooling rate during heat treatment can alter the balance of oxygen-related defects [6].

Studying the relationship between structural defects and electrical conductivity is essential for controlling the functional properties of ZnO thin films. By comparing crystal structure parameters - determined via XRD - with electrical measurement data, one can evaluate potential links between the structural state of a film and the transport of charge carriers. In this context, an increase in electrical conductivity does not necessarily imply a reduction in structural defects; for instance, a rise in charge carrier concentration may compensate for a decrease in mobility. Conversely, while improved crystalline order may enhance electron mobility, the overall electrical conductivity might not increase as expected if the charge carrier concentration simultaneously declines. Therefore, to accurately interpret the electrical properties of ZnO thin films, it is necessary to integrate structural analysis, electrical measurements, and - where possible - additional spectroscopic data regarding the nature of the defects.

There is no single, universal functional relationship between defect concentration and electrical conductivity (σ). For example, an increase in the number of electrically active donors may raise the carrier concentration n, yet this can also lead to enhanced scattering - whether from defects or grain boundaries - which in turn reduces mobility μ. Therefore, although an increase in annealing temperature may lead to improved crystallization and higher electrical conductivity, this is not a guaranteed trend for every ZnO sample.

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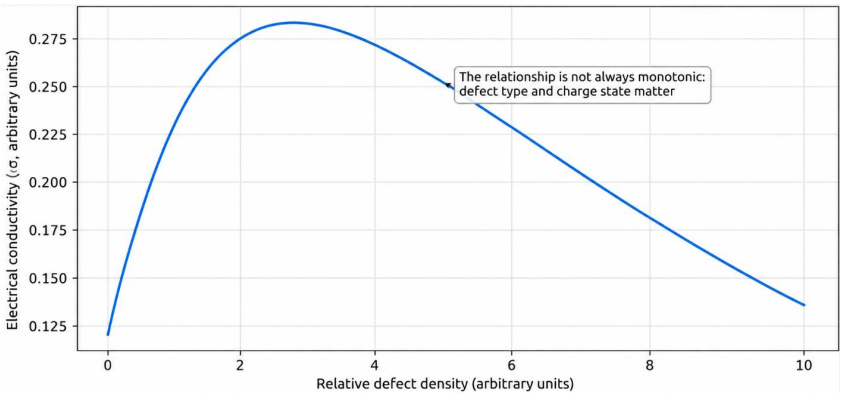


Figure 3. A conceptual, schematic relationship between defect density and conductivity. The curve does not represent experimental data; it merely illustrates that the relationship may not be monotonic due to the involvement of various mechanisms.

A single measurement technique is insufficient for the complete characterization of ZnO thin films. While XRD provides information on the crystalline phase, texture, lattice parameters, and the width of diffraction peaks, it does not always directly identify the chemical nature of a defect. Photoluminescence (PL) can reveal optical transitions and emission bands associated with defects; however, attributing a specific PL band to a single type of defect requires caution. The Hall effect measurement helps determine carrier concentration and mobility, while the four-probe method is used to assess electrical resistance.

When studying films prepared via the sol-gel and spin-coating method, one can keep parameters such as the precursor composition, number of layers, substrate type, and drying conditions constant, while systematically varying a single factor - for instance, the annealing temperature. As an example, conditions corresponding to 300, 400, and 500 °C can be compared. For each condition, it is recommended to prepare at least three replicate samples, measure the thickness, record the measurement uncertainty, and use the same contact geometry. This approach helps to isolate the effect of temperature from other process variables.

The primary advantage of an interdisciplinary approach lies in linking structural characteristics with electrical properties through complementary methods. For instance, the narrowing of XRD peaks may indicate an increase in crystallite size or a reduction in microstrain; meanwhile, an observed increase in mobility during Hall effect measurements suggests a potential decrease in scattering at grain boundaries. However, this conclusion cannot be substantiated by XRD data alone; factors such as film thickness, carrier concentration, surface adsorption, and contact resistance must also be examined.

If electrical conductivity increases following an annealing process, this could be attributed to an rise in electron concentration, an increase in mobility, or both. Conversely, a decrease in conductivity might stem from oxygen-related surface processes, the passivation of donors, the formation of compensating defects, or the emergence of barriers at grain boundaries. Therefore, rather than relying on a single-factor deduction - such as assuming that a reduction in defects automatically leads to higher conductivity - it is essential to compare results obtained from multiple independent measurements.

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CONCLUSION. This study focuses on a comprehensive investigation of the relationship between structural defects and electrical conductivity in ZnO thin films. Theoretical analysis indicates that the electrical conductivity of ZnO is determined by the concentration and mobility of charge carriers. These parameters, in turn, can be influenced by defects within the crystal lattice, grain boundaries, micro-strains, and thermal processing conditions. X-ray diffraction (XRD) serves as an essential tool for evaluating crystal structure, the broadening of diffraction peaks, and the estimated size of crystallites. However, to determine the concentration of specific types of defects, XRD results must be supplemented by electrical measurements and other relevant analytical techniques.

Comparing the structural and electrical properties of ZnO thin films enables a better understanding of how defects affect charge carrier transport and facilitates the selection of appropriate technological conditions for specific applications. Furthermore, variations in electrical conductivity cannot be attributed to a single type of defect; rather, the physical nature of the defects, their concentration, and the microstructure of the film must all be considered collectively. It is recommended to subsequently obtain XRD patterns for ZnO samples subjected to thermal treatment at various temperatures, measure their resistivity, charge carrier concentration, and mobility, and perform a statistical analysis of the quantitative relationships between these parameters. Such an approach facilitates the drawing of well-founded conclusions regarding the influence of structural defects on electrical conductivity and serves to optimize the characteristics of ZnO-based electronic and optoelectronic devices.

Conclusion. The electrical conductivity of ZnO thin films is determined by the type and charge state of structural defects, the concentration and mobility of charge carriers, grain boundaries, and surface processes. Depending on the conditions, defects can act as sources of electrons, or conversely, they may trap charge carriers or enhance scattering. Therefore, it is incorrect to assume a universal, monotonic relationship between defect density and conductivity. To draw reliable conclusions, it is necessary to integrate techniques such as XRD, PL, Hall effect measurements, and four-probe electrical measurements, while also controlling film thickness and morphology, and accounting for sample reproducibility and uncertainties. This approach - combining knowledge from crystallography, solid-state physics, surface chemistry, and electronics - facilitates the control of material properties for ZnO-based sensors and optoelectronic devices.

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