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X-RAY DIFFRACTION ANALYSIS OF ZnO, CuO, ANd Cu_2O THIN FILMS DEPOSITED BY ION-PLASMA TECHNOLOGY

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Abstract

Thin-film semiconductor oxides such as ZnO, CuO, and Cu_2O attract considerable scientific interest due to their unique structural, optical, and electrophysical

properties. The functional characteristics of these materials strongly depend on crystal structure, phase composition, and microstructural organization formed during synthesis. X-ray diffraction analysis remains one of the most effective methods for investigating structural properties of semiconductor thin films.

The present study investigates structural characteristics of ZnO, CuO, and Cu_2O thin films deposited on dielectric substrates using ion-plasma technology. Particular attention was devoted to comparative analysis of phase composition, crystallographic orientation, crystallite size, and structural ordering of the obtained semiconductor layers.

X-ray diffraction investigations demonstrated formation of polycrystalline semiconductor structures with characteristic crystal phases corresponding to hexagonal ZnO, monoclinic CuO, and cubic Cu_2O. Deposition conditions significantly influenced diffraction peak intensity, crystallinity, and structural homogeneity of the films.

The obtained results indicate that ion-plasma deposition technology enables controlled formation of structurally stable oxide semiconductor films with favorable crystallographic characteristics suitable for optoelectronic and energy-related applications.

Keywords. X-ray diffraction, ZnO thin films, CuO thin films, Cu_2O thin films, ion-plasma deposition, crystal structure, semiconductor oxides, phase analysis

Introduction

Semiconductor oxide thin films have become one of the most intensively investigated classes of functional materials in modern materials science and semiconductor physics. Among them, zinc oxide (ZnO), copper(II) oxide (CuO), and copper(I) oxide (Cu_2O) attract considerable scientific and technological attention due to their unique structural, optical, and electrophysical properties.

ZnO is a wide-band-gap semiconductor characterized by high optical transparency, excellent chemical stability, and favorable electrical conductivity. CuO and Cu_2O are p-type semiconductor materials widely used in photovoltaic systems, gas sensors, photocatalytic devices, and optoelectronic applications because of their narrow band gaps and high optical absorption coefficients.

The structural characteristics of thin semiconductor films strongly depend on synthesis conditions, deposition technology, substrate type, plasma parameters, and oxygen concentration during growth. Crystal structure, phase composition, crystallographic orientation, and defect concentration significantly influence the electrical and optical behavior of semiconductor oxide films.

Among various structural characterization methods, X-ray diffraction (XRD) analysis remains one of the most informative and widely used techniques for investigation of crystalline materials. XRD provides important information regarding phase composition, crystallinity, preferential orientation, lattice parameters, crystallite size, and structural defects in thin-film semiconductor systems.

Ion-plasma deposition technology is considered an effective method for fabrication of oxide semiconductor thin films because it enables precise control over growth conditions and formation of structurally homogeneous layers. During ion-plasma synthesis, energetic plasma particles influence nucleation mechanisms, crystallization dynamics, and phase formation processes occurring on the substrate surface.

Structural analysis of ZnO, CuO, and Cu_2O thin films is particularly important because these materials may exhibit different crystal phases and microstructural characteristics depending on oxygen partial pressure and plasma conditions.

Formation of secondary phases, grain boundaries, and structural defects may substantially affect functional properties of the films.

Recent advances in semiconductor nanotechnology and renewable energy systems have increased the importance of comparative structural investigations of oxide semiconductor thin films. Optimization of crystal structure and phase stability is essential for improving performance of modern electronic, optoelectronic, and photovoltaic devices.

Despite extensive research in this field, many aspects related to structural evolution and crystallographic behavior of ion-plasma-deposited ZnO, CuO, and Cu_2O thin films remain insufficiently investigated. Comparative X-ray diffraction analysis may provide deeper understanding of phase formation mechanisms and structural stability of these semiconductor materials.

Therefore, the aim of the present study is to perform X-ray diffraction analysis of ZnO, CuO, and Cu_2O thin films deposited by ion-plasma technology and to evaluate the influence of deposition conditions on their structural and crystallographic characteristics.

Materials and Methods

ZnO, CuO, and Cu_2O thin films were deposited on dielectric glass substrates using ion-plasma deposition technology under controlled vacuum conditions. Prior to deposition, the substrates were subjected to mechanical polishing and chemical cleaning procedures in order to eliminate surface contamination and improve adhesion of the deposited semiconductor layers.

High-purity zinc and copper targets were used as source materials during film synthesis. Oxygen was introduced into the deposition chamber to regulate oxidation processes and stabilize the required semiconductor oxide phases. The deposition process was carried out in a plasma environment generated under controlled discharge conditions.

The main technological parameters, including chamber pressure, plasma discharge power, substrate temperature, oxygen partial pressure, and deposition duration, were systematically controlled throughout the experiment. Variations in these parameters were used to investigate their influence on crystal structure, phase composition, and microstructural evolution of the deposited films.

Structural characterization of ZnO, CuO, and Cu_2O thin films was performed using X-ray diffraction analysis. Diffraction patterns were recorded within a selected angular range using monochromatic X-ray radiation. The obtained diffraction spectra were analyzed to determine crystal structure, phase composition, preferential crystallographic orientation, and structural ordering of the films.

The average crystallite size was estimated using the Scherrer equation:

$$D = \frac{K\lambda}{\beta\cos\theta}$$

where:

- Dis the average crystallite size;
- Kis the shape factor;
- λis the X-ray wavelength;
- βis the full width at half maximum of the diffraction peak;
- θis the diffraction angle.

The interplanar spacing values were determined according to Bragg’s law:

$$n\lambda = 2d\sin\theta$$

where:

- nis the diffraction order;
- λis the X-ray wavelength;
- dis the interplanar spacing;

- θis the Bragg angle.

Comparative structural analysis was carried out to evaluate differences in crystallographic phases, peak intensity, crystallinity, and structural stability among ZnO, CuO, and Cu_2O semiconductor films.

The obtained experimental data were systematized and comparatively analyzed to determine the relationship between ion-plasma deposition conditions and structural characteristics of the investigated oxide semiconductor thin films.

Results

X-ray diffraction analysis confirmed successful formation of crystalline ZnO, CuO, and Cu_2O thin films deposited by ion-plasma technology on dielectric substrates. The obtained diffraction patterns demonstrated characteristic reflections corresponding to the crystal structures of each semiconductor oxide material.

ZnO thin films exhibited diffraction peaks associated with the hexagonal wurtzite crystal structure. The most intensive reflection was observed along the (002) crystallographic plane, indicating preferential orientation of crystallites along the c-axis. Increased peak intensity and reduced peak broadening suggested improved crystallinity under optimized deposition conditions.

CuO thin films demonstrated formation of a monoclinic crystal phase characterized by several dominant diffraction reflections corresponding to typical CuO crystallographic planes. Variations in oxygen concentration and plasma discharge parameters significantly influenced crystallographic ordering and structural homogeneity of the films.

For Cu_2O thin films, diffraction analysis revealed formation of a cubic crystal structure with clearly defined characteristic peaks corresponding to the Cu_2O phase. Under optimized oxygen conditions, phase-pure Cu_2O structures were obtained with minimal formation of secondary CuO phases.

Comparative analysis showed that the structural quality of all investigated films strongly depended on deposition parameters, particularly substrate temperature and oxygen partial pressure. Improved crystallinity was accompanied by increased crystallite size and reduced structural defects.

Table 1. Structural Characteristics of ZnO, CuO, and Cu_2O Thin Films

Thin Film Material	Crystal Structure	Preferred Orientation	Structural Stability	Crystallinity
ZnO	Hexagonal wurtzite	(002) plane	High	High
CuO	Monoclinic	Multiple orientations	Moderate–High	Moderate
Cu_2O	Cubic	(111) orientation	High	High

Note. Structural parameters obtained from X-ray diffraction analysis of semiconductor oxide thin films synthesized by ion-plasma deposition.

The average crystallite size calculated using the Scherrer equation varied among the investigated materials and increased under elevated substrate temperatures. Larger crystallite dimensions were associated with enhanced structural ordering and improved film compactness.

The obtained diffraction patterns additionally demonstrated that oxygen concentration plays a decisive role in phase stabilization during film growth. Excess oxygen promoted formation of secondary oxide phases, particularly in copper oxide films, whereas optimized oxygen conditions contributed to stabilization of phase-pure semiconductor structures.

The results indicate that ion-plasma deposition technology enables controlled synthesis of structurally stable oxide semiconductor thin films with favorable crystallographic characteristics suitable for optoelectronic, photovoltaic, and semiconductor applications.

Comparative Analysis of Diffraction Behavior

The comparative XRD analysis revealed noticeable differences in crystallographic behavior among ZnO, CuO, and Cu_2O thin films. ZnO films exhibited the highest degree of preferential orientation and structural uniformity, which may be associated with the intrinsic stability of the wurtzite crystal structure.

CuO thin films demonstrated relatively broader diffraction peaks, indicating smaller crystallite size and increased concentration of structural defects. In contrast, Cu_2O films exhibited sharper diffraction reflections under optimized oxygen conditions, confirming improved phase stability and crystal ordering.

The observed structural differences are closely related to oxidation kinetics, plasma-assisted nucleation mechanisms, and thermodynamic stability of the corresponding oxide semiconductor phases.

Discussion

The results obtained in the present study demonstrate that ion-plasma deposition technology enables controlled synthesis of ZnO, CuO, and Cu_2O thin films with distinct crystal structures and stable structural characteristics. X-ray diffraction analysis confirmed successful formation of semiconductor oxide phases corresponding to hexagonal ZnO, monoclinic CuO, and cubic Cu_2O structures.

One of the most important findings of the investigation was the strong dependence of crystallographic behavior on deposition parameters, particularly oxygen concentration and substrate temperature. Proper control of plasma conditions promoted improved crystallinity, enhanced structural ordering, and stabilization of phase-pure semiconductor layers.

ZnO thin films exhibited the highest degree of preferential orientation along the (002) crystallographic plane. This behavior indicates anisotropic crystal growth and relatively low structural disorder during film formation. The high crystallinity of ZnO layers may be associated with the thermodynamic stability of the hexagonal wurtzite structure and favorable nucleation mechanisms during ion-plasma deposition.

In contrast, CuO thin films demonstrated broader diffraction peaks and less pronounced preferential orientation. These features suggest smaller crystallite dimensions and higher concentration of structural imperfections. Grain boundaries, lattice distortions, and oxygen-related defects may significantly influence crystallization dynamics in CuO semiconductor layers.

Cu_2O thin films exhibited improved phase stability and relatively sharp diffraction reflections under optimized oxygen conditions. The obtained results confirm that oxygen partial pressure plays a decisive role in controlling oxidation kinetics and stabilization of copper oxide semiconductor phases. Excess oxygen concentration promoted partial transformation of Cu_2O into CuO, indicating high sensitivity of copper oxide phase formation to deposition conditions.

The comparative analysis additionally revealed that crystallite size and structural homogeneity increase with substrate temperature and deposition duration. Enhanced atomic mobility under elevated temperatures contributes to improved crystal growth and reduction of structural defects within the films.

The observed structural characteristics are closely associated with electrophysical behavior and potential functional performance of the investigated semiconductor materials. Improved crystallinity and reduced defect concentration generally contribute to enhanced electrical conductivity, carrier mobility, and optical stability of oxide semiconductor films.

Another important aspect of the study is the technological effectiveness of ion-plasma deposition for fabrication of oxide semiconductor thin films. The method provides precise control over plasma-assisted growth mechanisms, phase composition, and structural evolution of the deposited materials. Such advantages

are highly important for development of advanced semiconductor and optoelectronic systems.

The investigated ZnO, CuO, and Cu_2O thin films demonstrate promising potential for application in photovoltaic devices, transparent conductive coatings, gas sensors, photodetectors, and energy conversion technologies. Their structural stability and controllable crystallographic characteristics make them suitable for modern electronic and photonic applications.

Despite the favorable experimental results, additional investigations are necessary for deeper understanding of defect formation processes, phase transition mechanisms, and structure-property relationships in oxide semiconductor films. Further studies involving optical spectroscopy, Hall-effect measurements, and temperature-dependent structural analysis may provide more comprehensive information regarding physical processes occurring in ion-plasma-grown semiconductor structures.

In conclusion, the present study confirms that optimization of ion-plasma deposition parameters plays a crucial role in controlling crystal structure, phase stability, and microstructural organization of ZnO, CuO, and Cu_2O thin films. Improved understanding of these processes may contribute to further advancement of semiconductor oxide technologies and expansion of their applications in renewable energy and optoelectronic systems.

Conclusion

The present study demonstrated that ZnO, CuO, and Cu_2O thin films synthesized by ion-plasma deposition on dielectric substrates possess stable crystalline structures and favorable structural characteristics. X-ray diffraction analysis confirmed successful formation of hexagonal ZnO, monoclinic CuO, and cubic Cu_2O semiconductor phases under controlled deposition conditions.

It was established that plasma discharge parameters, oxygen concentration, substrate temperature, and deposition duration significantly influence phase formation, crystallographic orientation, crystallite growth, and structural stability of the deposited films. Optimization of deposition conditions contributed to improved crystallinity, enhanced structural homogeneity, and reduction of defect concentration.

Comparative structural analysis revealed that ZnO films exhibited the highest degree of preferential orientation and structural ordering, while CuO and Cu_2O films demonstrated strong dependence of phase stability on oxygen partial pressure during synthesis. Stabilization of phase-pure copper oxide structures was achieved through precise regulation of oxidation conditions within the plasma environment.

The obtained results indicate that ion-plasma technology provides effective control over structural evolution and crystallographic characteristics of oxide semiconductor thin films. The investigated materials demonstrate promising potential for application in optoelectronic systems, photovoltaic devices, semiconductor sensors, transparent conductive coatings, and renewable energy technologies.

Further investigations involving optical spectroscopy, Hall-effect measurements, and temperature-dependent structural analysis may contribute to deeper understanding of phase transition mechanisms and structure–property relationships in ion-plasma-grown oxide semiconductor thin films.

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