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INFLUENCE OF CRYSTALLITE SIZE ON THE ELECTRICAL PROPERTIES OF ZNO AND CUO THIN FILMS

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Abstract

The structural characteristics of semiconductor thin films play a crucial role in determining their electrical and functional behavior. Among various microstructural parameters, crystallite size significantly influences charge transport mechanisms, carrier mobility, grain boundary effects, and electrical conductivity of oxide semiconductor materials. ZnO and CuO thin films are widely used in optoelectronic devices, photovoltaic systems, sensors, and nanoelectronic technologies due to their favorable semiconductor properties.

The present study investigates the influence of crystallite size on the electrical properties of ZnO and CuO thin films deposited on dielectric substrates using ion-plasma technology. Particular attention was devoted to the relationship between structural ordering, grain growth, electrical resistivity, and conductivity mechanisms of the synthesized films.

The obtained results demonstrated that increased crystallite size contributes to reduced grain boundary scattering and improved electrical conductivity of both ZnO and CuO thin films. Films characterized by enhanced crystallinity and larger grain dimensions exhibited lower electrical resistivity and more stable charge transport behavior.

The study confirms that optimization of deposition parameters and control of crystallite growth are essential for improving electrophysical performance of oxide semiconductor thin films intended for modern electronic and optoelectronic applications.

Keywords: ZnO thin films, CuO thin films, crystallite size, electrical conductivity, electrophysical properties, ion-plasma deposition, semiconductor oxides, grain boundary effects.

Introduction

The electrical properties of semiconductor thin films are strongly influenced by their structural and microstructural characteristics. Among these parameters,

crystallite size plays a particularly important role in determining charge carrier transport, electrical conductivity, carrier mobility, and grain boundary scattering mechanisms. Control of crystallite growth is therefore considered one of the key factors in optimization of semiconductor materials for electronic and optoelectronic applications.

ZnO and CuO thin films are widely investigated oxide semiconductor materials due to their favorable optical, electrical, and chemical properties. ZnO is a wide-band-gap n-type semiconductor characterized by high transparency and stable conductivity, while CuO is a narrow-band-gap p-type semiconductor with strong optical absorption and promising photoelectrical behavior.

The functional performance of these materials strongly depends on synthesis technology and deposition conditions. Structural defects, grain boundaries, crystallographic orientation, and crystallite dimensions significantly influence electrical transport processes within semiconductor thin films.

Among modern fabrication techniques, ion-plasma deposition technology provides substantial advantages for controlling microstructural organization of semiconductor layers. Plasma-assisted deposition enables precise regulation of crystallization processes, grain growth, and structural homogeneity of the synthesized films.

The relationship between crystallite size and electrical conductivity is mainly associated with grain boundary effects. In polycrystalline semiconductor films, grain boundaries act as scattering centers that limit carrier mobility and increase electrical resistance. Enlargement of crystallite dimensions reduces the number of grain interfaces and facilitates more efficient charge transport within the semiconductor structure.

Previous studies have shown that increased crystallinity and larger grain size generally contribute to improved conductivity characteristics and reduced resistive losses in oxide semiconductor films. However, the influence of crystallite growth on electrophysical behavior may vary depending on material composition, defect concentration, and deposition conditions.

Recent advances in nanotechnology and semiconductor engineering have intensified research aimed at optimization of microstructural parameters of ZnO and CuO thin films for photovoltaic systems, gas sensors, transparent conductive coatings, and nanoelectronic devices.

Despite extensive investigations of oxide semiconductor materials, many aspects related to the correlation between crystallite size and electrical transport behavior in ion-plasma-deposited films remain insufficiently studied. Detailed understanding of these relationships is essential for development of highly efficient semiconductor technologies.

Therefore, the aim of the present study is to investigate the influence of crystallite size on the electrical properties of ZnO and CuO thin films synthesized by ion-plasma deposition and to evaluate the role of grain growth in charge transport mechanisms of oxide semiconductor structures.

Materials and Methods

ZnO and CuO thin films were deposited on dielectric glass substrates using ion-plasma deposition technology under controlled laboratory conditions. Prior to deposition, the substrates were mechanically polished and chemically cleaned to remove impurities and improve adhesion of the semiconductor layers.

High-purity zinc and copper targets were used as source materials during film synthesis. Oxygen gas was introduced into the vacuum chamber in order to regulate oxidation processes and stabilize formation of ZnO and CuO semiconductor phases. The deposition process was carried out in a plasma environment generated under controlled discharge parameters.

The main technological parameters, including plasma discharge power, oxygen partial pressure, substrate temperature, chamber pressure, and deposition duration, were systematically controlled during film growth. Variations in these parameters allowed regulation of crystallite size and microstructural characteristics of the deposited films.

Structural characterization was performed using X-ray diffraction analysis. Diffraction patterns were recorded to determine crystal structure, crystallinity, and average crystallite size of ZnO and CuO thin films. The average crystallite dimensions were estimated using the Scherrer equation:

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

where:

- $D$is the average crystallite size;
- $K$is the shape factor;
- $\lambda$is the X-ray wavelength;
- $\beta$is the diffraction peak broadening;
- $\theta$is the Bragg diffraction angle.

Electrical conductivity measurements were carried out at room temperature using standard electrical characterization techniques. The electrical resistivity of the deposited films was calculated according to the relation:

$$\rho = R\frac{A}{l}$$

where:

- $\rho$is electrical resistivity;
- $R$is electrical resistance;
- $A$is the cross-sectional area of the sample;
- $l$is the distance between electrical contacts.

Comparative analysis was performed to evaluate the relationship between crystallite size, structural ordering, and electrical conductivity behavior of ZnO and CuO thin films. Special attention was devoted to the influence of grain boundaries and defect concentration on charge transport mechanisms within the semiconductor structures.

Results

X-ray diffraction analysis confirmed successful formation of polycrystalline ZnO and CuO thin films with characteristic crystal structures corresponding to hexagonal ZnO and monoclinic CuO phases. Variations in deposition parameters significantly influenced crystallite size, structural ordering, and electrical properties of the deposited semiconductor layers.

The calculated crystallite size increased with substrate temperature and deposition duration for both ZnO and CuO films. Enhanced crystallite growth was accompanied by improved crystallinity and reduction of structural defects within the semiconductor structures.

ZnO thin films exhibited relatively larger crystallite dimensions and stronger preferential orientation compared with CuO films. Increased crystallite size contributed to improved electrical conductivity due to reduction of grain boundary scattering effects and enhanced carrier mobility.

CuO thin films demonstrated similar behavior, although the influence of structural defects and grain interfaces on electrical transport was more pronounced. Films characterized by smaller crystallite size exhibited increased electrical resistance due to higher concentration of grain boundaries acting as carrier scattering centers.

Electrical measurements revealed that electrical resistivity decreased with increasing crystallite size for both investigated semiconductor materials. Larger grains reduced the number of grain interfaces and facilitated more efficient charge transport through the films.

Table 1. Influence of Crystallite Size on Electrical Properties of ZnO and CuO Thin Films

Thin Film Material	Crystallite Size Trend	Electrical Resistivity	Conductivity Behavior
ZnO	Increased with temperature	Decreased	Improved conductivity
CuO	Increased with deposition time	Decreased	Enhanced charge transport

Note. Comparative relationship between crystallite growth and electrical characteristics of oxide semiconductor thin films.

The obtained results indicate that crystallite size plays a decisive role in determining electrical transport mechanisms in polycrystalline semiconductor films. Improved structural ordering and reduced grain boundary concentration contribute to enhanced carrier mobility and lower resistive losses.

The relationship between grain size and electrical conductivity may be explained by the reduction of carrier scattering processes occurring at grain interfaces. Larger crystallites provide more continuous pathways for charge transport and improve electrophysical stability of the semiconductor layers.

Charge Transport Mechanism

Electrical conductivity in polycrystalline oxide semiconductor films is strongly influenced by grain boundary effects. The electrical resistance associated with grain interfaces may be expressed as:

$$\sigma = nq\mu$$

where:

- σ is electrical conductivity;
- n is carrier concentration;
- q is the elementary charge;
- μ is carrier mobility.

Increase in crystallite size contributes to higher carrier mobility by reducing scattering effects at grain boundaries and structural defects.

Discussion

The results obtained in the present study demonstrate that crystallite size significantly influences the electrical properties of ZnO and CuO thin films synthesized by ion-plasma deposition technology. Structural investigations confirmed that optimization of deposition conditions promotes crystallite growth, improves crystallinity, and enhances electrophysical behavior of oxide semiconductor films.

One of the most important findings of the study was the reduction of electrical resistivity with increasing crystallite size for both ZnO and CuO semiconductor layers. This behavior may be explained by the decrease in grain boundary density within the films. Grain boundaries act as potential barriers and carrier scattering centers that limit charge transport efficiency in polycrystalline semiconductor materials.

ZnO thin films exhibited relatively higher crystallinity and larger crystallite dimensions compared with CuO films. The strong preferential orientation observed in ZnO layers contributed to more stable conductivity and improved carrier mobility. Reduced structural disorder facilitated more effective electron transport through the semiconductor structure.

CuO thin films also demonstrated enhanced electrical conductivity with increasing crystallite size, although the influence of grain interfaces and structural defects remained more pronounced. The narrower band gap and complex defect structure of CuO semiconductor layers may contribute to stronger carrier scattering processes and higher sensitivity to microstructural imperfections.

The obtained results confirm that crystallite growth is closely associated with improved structural ordering and reduction of defect concentration. Increased substrate temperature and optimized plasma conditions promote atomic diffusion on the substrate surface and facilitate formation of larger grains with enhanced structural stability.

The observed dependence of conductivity on crystallite dimensions is consistent with theoretical models describing charge transport mechanisms in polycrystalline semiconductor films. Reduction of grain boundary barriers improves carrier mobility and decreases resistive losses within the material.

Another important aspect of the study is the effectiveness of ion-plasma deposition technology for controlling microstructural characteristics of semiconductor oxide films. The method enables precise regulation of plasma-assisted nucleation processes, grain growth dynamics, and structural evolution during thin-film synthesis.

The investigated ZnO and CuO thin films demonstrate promising potential for application in optoelectronic systems, gas sensors, photovoltaic technologies, transparent conductive coatings, and nanoelectronic devices. Optimization of crystallite size and structural homogeneity may significantly improve performance and operational stability of such semiconductor systems.

Despite the favorable experimental results, additional investigations remain necessary for deeper understanding of defect-related conductivity mechanisms and carrier transport processes in oxide semiconductor films. Future studies involving Hall-effect measurements, temperature-dependent conductivity analysis, and advanced microscopic characterization may provide more comprehensive

information regarding the influence of microstructural parameters on electrical behavior.

In conclusion, the present study confirms that crystallite size is one of the key factors determining electrophysical properties of ZnO and CuO thin films. Control of grain growth through optimization of ion-plasma deposition parameters may contribute to further advancement of semiconductor oxide technologies and expansion of their practical applications in modern electronic and photonic systems.

Conclusion

The present study demonstrated that crystallite size has a substantial influence on the electrical properties of ZnO and CuO thin films deposited on dielectric substrates by ion-plasma technology. Structural analysis confirmed that optimization of deposition parameters contributes to crystallite growth, improved crystallinity, and enhanced structural homogeneity of the semiconductor layers.

It was established that increased crystallite size leads to reduced grain boundary scattering and lower electrical resistivity in both ZnO and CuO thin films. Improved crystal ordering facilitated more efficient charge transport and enhanced carrier mobility within the semiconductor structures.

ZnO films exhibited relatively higher crystallinity and more stable conductivity characteristics, while CuO films demonstrated stronger dependence of electrical behavior on structural defects and grain interface effects. The obtained results confirmed that microstructural organization plays a decisive role in determining electrophysical performance of oxide semiconductor materials.

The study additionally demonstrated that ion-plasma deposition technology provides effective control over crystallization dynamics and microstructural evolution of semiconductor thin films. Regulation of substrate temperature, oxygen

concentration, and plasma discharge parameters enables fabrication of oxide films with optimized electrical characteristics.

The investigated ZnO and CuO thin films exhibit promising potential for application in optoelectronic systems, photovoltaic devices, transparent conductive coatings, gas sensors, and semiconductor nanoelectronics. Optimization of crystallite dimensions may significantly improve functional performance and operational stability of semiconductor oxide technologies.

Further investigations involving Hall-effect analysis, temperature-dependent conductivity measurements, and advanced microscopic characterization may contribute to deeper understanding of charge transport mechanisms and defect-related phenomena in oxide semiconductor thin films.

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