Data-Driven Gas Sensing Analysis of Ag-Doped Cdo Thin Films

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Abstract: Pure and Ag-doped CdO thin films were successfully synthesized using the chemical spray pyrolysis (CSP) technique. The influence of silver doping on the structural, morphological, optical, and gas-sensing properties of CdO films was systematically investigated. X-ray diffraction analysis confirmed the formation of polycrystalline CdO films with a preferred orientation along the (111) plane. An increase in crystallite size from 17.78 nm for pure CdO to 23.55 nm for 4% Ag-doped CdO was observed, accompanied by a reduction in dislocation density and microstrain, indicating improved crystalline quality. Atomic force microscopy revealed smoother and more compact surfaces with increasing Ag concentration. Optical investigations in the wavelength range of 300–900 nm demonstrated a decrease in transmittance and a narrowing of the optical bandgap from 2.65 eV to 2.55 eV as the Ag doping level increased. The observed bandgap reduction was attributed to the formation of localized impurity states within the CdO lattice. Furthermore, the extinction coefficient and refractive index were found to vary significantly with Ag incorporation. Gas-sensing measurements toward NO_2 gas indicated that pure CdO films exhibited higher sensitivity compared to Ag-doped samples. The reduction in sensitivity with increasing Ag concentration was associated with enhanced charge-carrier recombination and a decrease in active adsorption sites on the film surface. The obtained results demonstrate that Ag doping effectively modifies the physical properties of CdO thin films and influences their suitability for gas-sensing applications.

1 INTRODUCTION

CdO is of which is a transparent conducting oxide with a bandgap in the range of 2.2 to 2.7 eV and at the same time, has very good electrical conductivity; thus is a material that has drawn attention for use in a wide variety of optoelectronics like, photodiodes, and flat panel displays [1]-[4]. CdO has a rock salt cubic structure which is very chemically stable and also reports high carrier mobility [3], [5]. But we see that pure CdO thin films exhibit a high defect density and relatively low transparency in the visible spectrum. To improve on this, we have seen that transition-metal doping is a widely used method for tuning the physical properties of CdO. Silver (Ag) is very promising, which we put down to its similar ionic radius to Cd^{2+}, high oxidation state (Ag^{4+} and also its ability to increase carrier concentration without greatly disturbing the lattice [6]. Also, the deposition technique used plays a very large role in the quality of CdO thin film [7], [8]. Many methods were used to produce CdO films., like CBD [9], sol-gel methods [10], SILAR [7], [10]-[12], CVD [13], magnetron sputtering [14]-[16], PLD [17], [18], VE [19] and CSP [20]-[22]. CSP stands out as a simple, cost-effective, [19]. CSP also enables large-area deposition with excellent uniformity and reproducibility [21]. Therefore, the present work aims to synthesize pure and Ag-doped CdO films via CSP method. The impact of Ag doping concentration on optical caharacterization is systematically discussed.

2 EXPERIMENTAL

Thin films of CdO: Ag we used the CSP method for growth. We prepared the intended films by dissolving 0.1 M of $CdCl_2 \cdot 6H_2O$ in 100 ml of DI. The volume ratio of the silver was 2% and 4%. In this work, we achieved the following results: we used a substrate temperature of 400 ºC. We sprayed the solution onto glass substrates that had undergone a cleaning process. Spray rate of 0.2 mL/s, spray-to-base distance of 28 cm, spray duration of 10 sec, 2 min interval between sequential sprayers, and N_2 as carrier gas at a pressure of 10^5 Pa. We determined film thickness by the gravimetric method which reported values in the range of 330±30 nm. We used a Shimadzu Japan double beam spectrophotometer to determine the transmittance. Also, we looked at the structural properties via XRD, we carried out gas sensing in a which we designed to be a cylinder of 7.5 cm radius and 15 cm height.

3 RESULTS AND DISCUSSIONS

The XRD patterns of the prepared films are presented in Figure 1. Diffraction peaks observed at 33.86°, 38.71°, and 66.15° correspond to the (111), (200), and (311) crystallographic planes, respectively, matching the ICDD card No. 30-065-2908. The results confirm the formation of polycrystalline CdO films with a preferred orientation along the (111) plane, in agreement with previous studies [23], [24].

The crystallite size was found to increase from 14.78 nm for pure CdO films to 23.55 nm for films doped with 4% Ag [25], [26]. This increase suggests an improvement in crystalline quality, which may be attributed to enhanced atomic diffusion and grain growth during film formation [27], [28].

In addition, the dislocation density decreased with increasing Ag concentration, dropping from 72.56 to 41.20, which indicates a reduction in lattice imperfections and structural defects [29], [30]. The incorporation of Ag ions appears to enhance crystal ordering and structural stability by promoting grain growth and reducing defect concentration [31], [32].

A similar trend was observed for microstrain values, which decreased from 28.47 to 21.81 with increasing Ag content. The reduction in microstrain indicates lower lattice distortion and internal stress, further confirming the improvement in crystallinity after Ag incorporation [33], [34]. Figure 2 summarizes the variation of FWHM, crystallite size, dislocation density, and microstrain as a function of Ag doping concentration.

Figure 3 presents the three-dimensional AFM topography images of the deposited films. The results reveal a systematic decrease in average particle size and surface roughness with increasing Ag concentration. Furthermore, the root-mean-square roughness decreased significantly from 7.86 nm to 4.09 nm as the Ag content increased. These changes suggest that Ag incorporation suppresses excessive grain growth and contributes to the formation of smoother and more uniform film surfaces [35], [36].

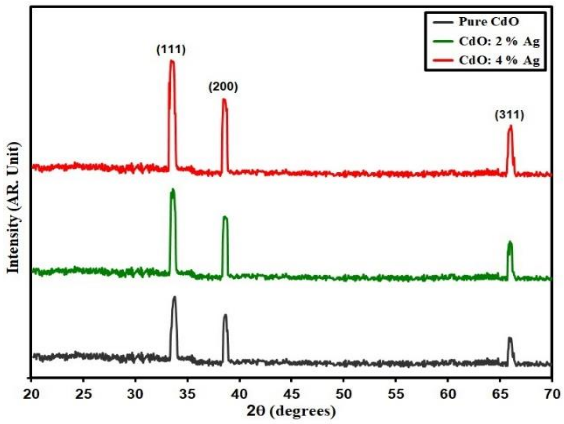

Figure 1: XRD patterns of pure and Ag-doped CdO thin films.

Table 1: Surface morphology parameters of pure and Ag-doped CdO thin films obtained from AFM analysis.

Specimen	A_P nm	Ra nm	Rms nm
CdO	73.8	8.31	7.86
CdO: 2% Ag	66.7	7.84	5.37
CdO: 4% Ag	55.9	3.66	4.09

Table 2: Structural and optical parameters of pure and Ag-doped CdO thin films derived from XRD analysis.

Sample	(hkl) Plane	2 □ (°)	FWHM (°)	Eg eV	D nm	□ × 10^{14} lines/m	ε× 10^{-4}
Pure CdO	111	33.86	0.79	2.65	17.78	72.56	28.47
CdO: 2% Ag	111	33.83	0.75	2.60	18.43	55.00	25.76
CdO: 4% Ag	111	33.80	0.71	2.55	23.55	41.20	21.81

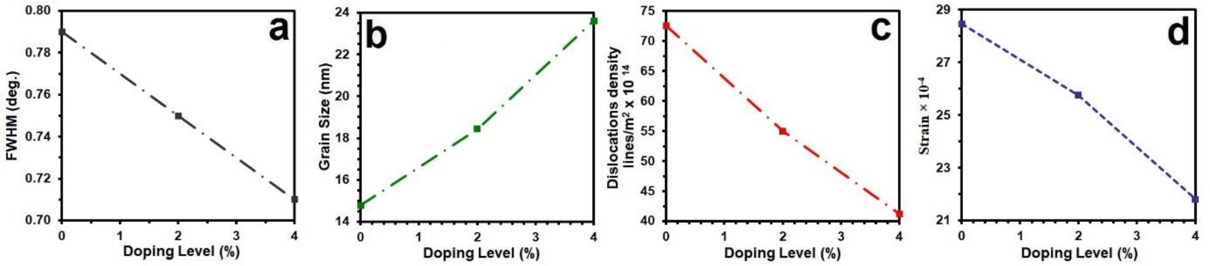

Figure 2: Variation of structural parameters of pure and Ag-doped CdO thin films.

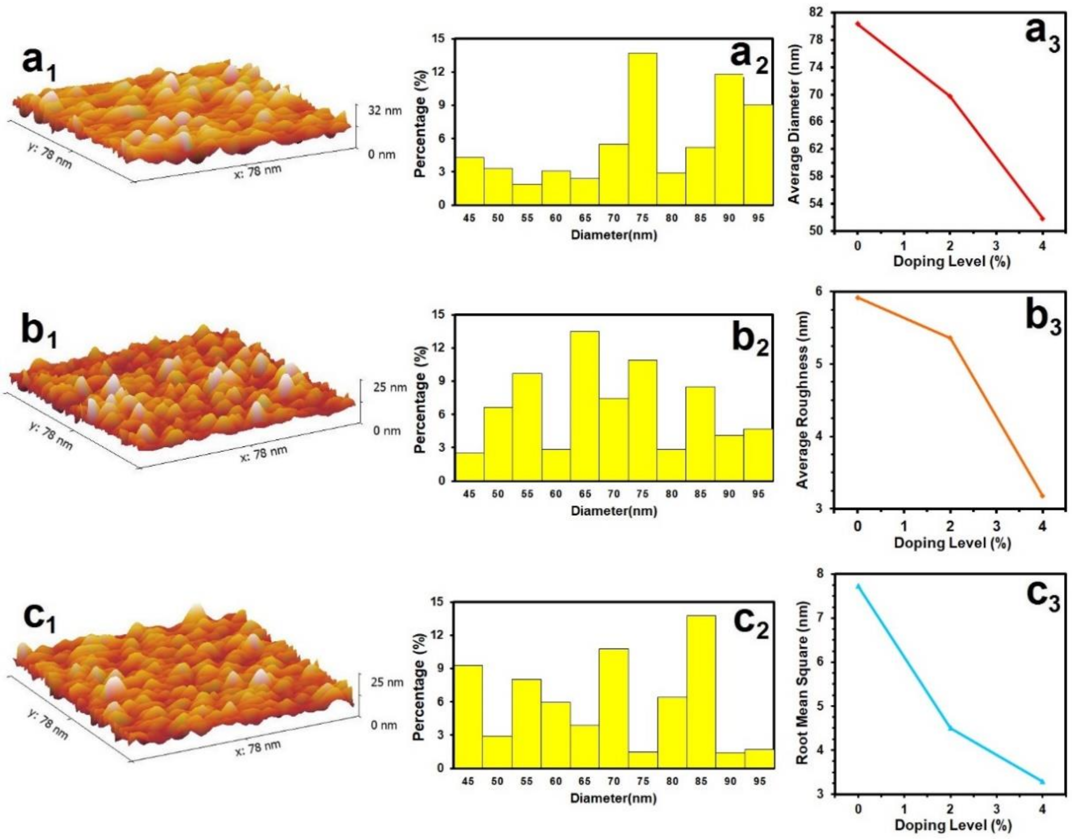

Figure 3: Three-dimensional AFM topography images of pure and Ag-doped CdO thin films.

Figure 4 illustrates the optical transmittance spectra of the prepared films. A gradual decrease in transmittance was observed with increasing Ag doping concentration [37]. This reduction in transparency can be attributed to enhanced light absorption and increased scattering caused by structural defects and impurity states introduced by Ag incorporation into the CdO lattice [38], [39].

Figure 5 presents the variation of the absorption coefficient for pure and Ag-doped CdO films. The absorption coefficient increased with increasing Ag concentration, indicating stronger photon absorption in the doped films [40], [41]. This behavior is associated with the formation of localized electronic states within the band structure, which enhance light–matter interaction and facilitate optical transitions [42].

The optical bandgap values [43] were found to decrease as the Ag doping level increased. Pure CdO films exhibited a bandgap of 2.65 eV, while films doped with 4% Ag showed a reduced value of 2.55 eV. The narrowing of the bandgap can be explained by the introduction of impurity levels and defect states resulting from Ag incorporation into the CdO crystal lattice [44], [45]. The corresponding optical transition behavior is illustrated in Figure 6.

Figure 7 shows the variation of the extinction coefficient with Ag concentration [46], [47]. A decrease in the extinction coefficient was observed as the Ag content increased [48], [49]. This trend suggests a reduction in optical attenuation and energy loss within the films, which may be related to modifications in the electronic structure and absorption characteristics caused by Ag doping [50], [51].

The refractive index behavior of the prepared films is presented in Figure 8. The refractive index decreased with increasing Ag concentration, which may be associated with changes in film density and microstructure [52], [54]. These structural modifications influence the dielectric properties and optical response of the CdO films [53], [55].

The gas-sensing performance of the films toward NO_2 gas was also investigated. Figure 9 presents the resistance variation of the films as a function of exposure time [56], [57]. Upon exposure to NO_2 gas, the resistance increased due to interactions between the gas molecules and adsorbed oxygen species on the CdO surface, leading to electron trapping and changes in charge transport properties [58], [59]. Among all investigated samples, the film doped with 4% Ag exhibited the highest resistance values, indicating enhanced gas interaction characteristics [60], [61].

Figure 10 demonstrates the influence of Ag doping on the NO_2 sensing response. The sensitivity decreased with increasing Ag concentration, mainly due to enhanced charge-carrier recombination and the reduction of active adsorption sites on the film surface. The sensitivity values decreased from 44.3% to 12.16% at 90 ppm, from 46.16% to 13.09% at 180 ppm, and from 48.69% to 15.88% at 270 ppm for pure CdO, 2% Ag-doped CdO, and 4% Ag-doped CdO films, respectively [62]-[64].

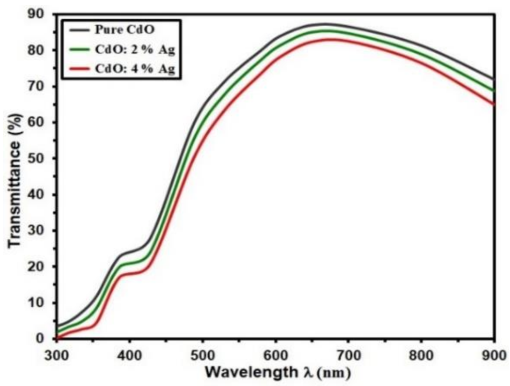

Figure 4: Optical transmittance spectra of pure and Ag-doped CdO thin films at different wavelengths.

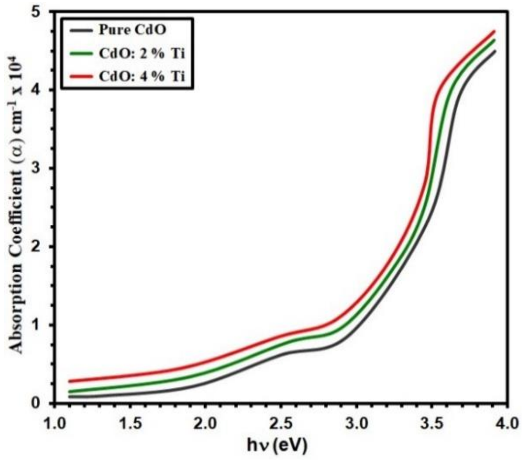

Figure 5: Absorption coefficient spectra of pure and Ag-doped CdO thin films.

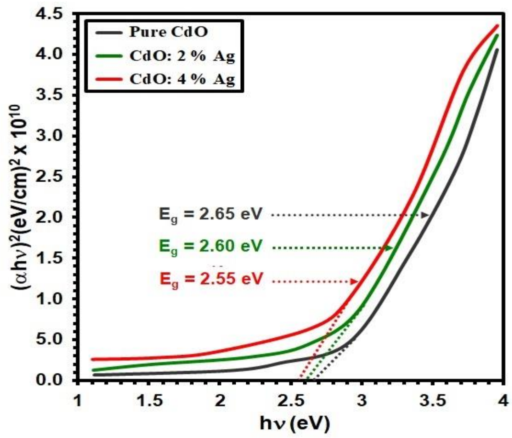

Figure 6: Optical bandgap plots of pure and Ag-doped CdO thin films.

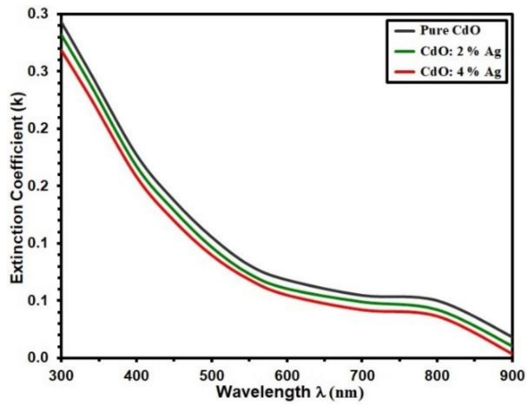

Figure 7: Extinction coefficient variation of pure and Ag-doped CdO thin films.

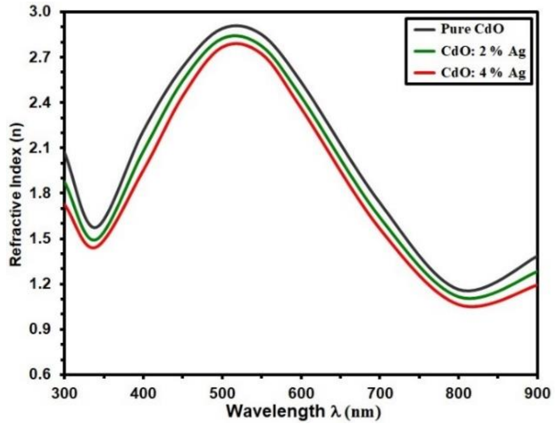

Figure 8: Variation of refractive index for pure and Ag-doped CdO thin films.

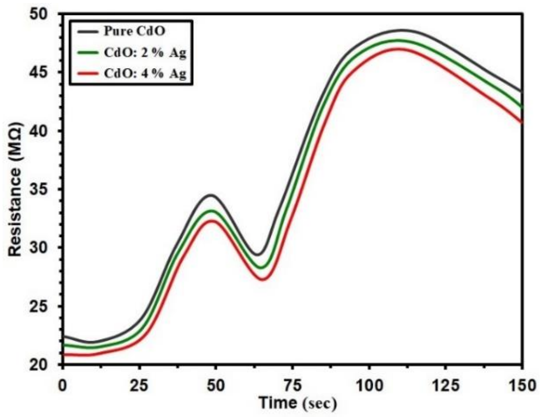

Figure 9: Resistance via time deposit films.

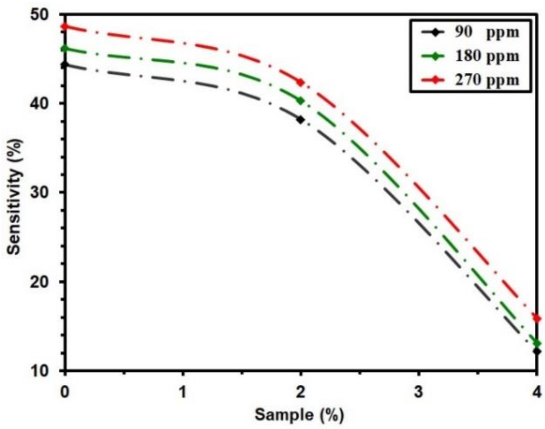

Figure 10: Sensitivity (S) of the intended films.

4 CONCLUSIONS

In this study, pure and Ag-doped CdO thin films were successfully synthesized using the chemical spray pyrolysis technique. Structural analysis confirmed the formation of polycrystalline CdO films with a preferred orientation along the (111) plane. Ag incorporation improved the crystalline quality of the films, as evidenced by the increase in crystallite size from 17.78 nm to 23.55 nm and the reduction in dislocation density and microstrain.

Morphological investigations revealed that Ag doping reduced the surface roughness and average particle size, resulting in smoother and more uniform film surfaces. Optical measurements demonstrated that increasing Ag concentration led to lower transmittance and a reduction in the optical bandgap from 2.65 eV to 2.55 eV, which was attributed to the formation of localized impurity states within the CdO lattice.

Gas-sensing measurements toward NO_2 gas showed that Ag doping significantly influenced the sensing behavior of CdO films. Although the electrical resistance increased with Ag concentration, the overall gas sensitivity decreased due to enhanced charge-carrier recombination and the reduction of active adsorption sites.

Overall, the obtained results indicate that Ag doping effectively modifies the structural, optical, and sensing properties of CdO thin films, making these materials promising candidates for optoelectronic and gas-sensing applications.

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