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DETERMINATION OF OPTICAL CONSTANTS OF CdO THIN FILMS DEPOSITED BY SOL-GEL SPIN COATING TECHNIQUE

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Abstract

The CdO thin films were synthesized on a glass substrate at room temperature with different molar concentrations of cadmium acetate using the sol-gel spin coating method. The sol-gel spin coating method is one of the most promising methods due to the simplicity of deposition, and low cost of the used materials and equipment. Which delivers high-homogeneity thin films at room temperature. The X-ray diffraction (XRD) study showed that all the films exhibited polycrystalline structures with cubic phases. The average crystallite size of the CdO films slightly decreased with an increase in the molar concentration of Cd. The values of the crystallite size of the films were found to be in the range of 14-15 nm. The decrease in size results in an increase in the defects in the deposited thin films. The lattice constant of CdO thin films is the same. The volume of the unit cell slightly changes with different concentrations. The transmission and absorbance spectra of the prepared films were measured using a UV-vis spectrophotometer in the wavelength range of 400-1100 nm. All films have a uniform pattern of absorption. They show lower absorption in the higher wavelength region. The optical bandgap was evaluated by the Tauc method. The optical band gap decreased from 3.06 to 2.1 eV depending on the concentration. The extinction coefficient (k), and refractive index (n) were determined. The extinction coefficient has the highest value for 0.5 M CdO thin films at a lower wavelength and its value decreased with increasing the molar concentration. The extinction coefficient computes the amount of light loss owing to scattering and absorption per unit volume of penetrating medium. The refractive index varies from 2.33 to 2.66 with decreasing molar concentration of Cd in CdO thin films. Refractive index changes also account for crystallite size and internal strain of the film.

Keywords: thin films, optoelectronic devices, cadmium oxide, spin coating

1. Introduction

The n-type degenerate semiconductor cadmium oxide (CdO) has a high electrical conductivity (10^2 - 10^4 Ω cm). CdO films have a direct bandgap between 2.2 and 2.7 eV and are transparent in the visible and near-infrared spectrums [1-4]. Consequently, there has been a considerable amount of interest in using CdO material in both its pure and doped states for optoelectronic applications such as solar cells, flat panel displays, optical communications, photo-transistors, and transparent conducting oxide, in addition to other types of applications like IR heat mirrors, gas sensors, low-emissive windows, and thin-film resistors, etc. [5-9]. The variation in electrical and optical properties can be attributed to the preparation process and the type of dopant utilized.

Various processes such as chemical bath deposition, magnetron sputtering, hydrothermal synthesis, pulsed laser deposition (PLD), and spray pyrolysis are reported to have prepared CdO films [10–14]. Among these techniques for thin film preparation, the sol-gel spin coating method is one of the most promising methods due to the simplicity of deposition, and low cost of the used materials and equipment. This method allows for the production of larger film areas and allows for the customization of thin film properties according to device specifications. Because the spin coating process is compatible with future optoelectronic devices that are produced using a low-cost solution method, we are using it here to fabricate thin films of CdO. The luminescence, photocatalytic, and electrical properties of the nanoparticles have improved recently. In earlier studies, the main focus was on the structural, optical, electrical, and optoelectrical properties of CdO. However, some experimental studies related to linear and nonlinear optical parameters such as refractive index, susceptibility, dielectric constant, etc. are absent. The main objective of this work is to elucidate the influence on linear, and optical characteristics of CdO films by spin coating. The prepared films have been investigated spectroscopically by using XRD, and UV-Vis absorption spectra. Various linear optical parameters such as optical band gap, refractive index, etc. have also been extracted from these results.

2. Experimental arrangement

2.1 Film preparation

We have chosen substrates of commercial-quality microscopic glass slides. Initially, they were dipped in nitric acid for 24 hours. After detergent wash, placed in an ultrasonic cleaner with triple distilled water and finally dried at room temperature. CdO thin films have been coated on the substrates through a sol-gel spin coating process using a spin coater. For the preparation of the CdO solutions, 0.5M and 1M of cadmium-acetate di-hydrate ($\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$) was dissolved in 2-methoxy ethanol and stirred by magnetic stirrer for 20 minutes at 27°C. The temperature of the plate was gradually ramped up to 70 °C then the stabilizer mono-ethanolamine was added drop-by-drop to the solutions. The obtained solutions and the mixtures were stirred for 2 hours to become homogeneous, and transparent solutions. The temperature of the final solutions and mixtures was reduced to room temperature. After that prepared solution was spread on a glass slide in spin coater equipment. The coated thin films were baked at 200°C for 15 minutes in the furnace to get rid of the solvents and organic contamination. The procedures from coating to drying were done repeatedly six times.

2.2 Measuring Instruments

The Optical absorption and transmission spectra for all deposited films were recorded over the wavelength range of 400–1100 nm using UV–Vis spectrophotometer CHEMITO SPECTRASCAN-2600. The photoluminescence spectra of the deposited films were recorded using a constant deviation spectrometer over the visible range of 400–700 nm. The X-ray diffraction patterns for the structural properties of prepared films were examined by using XPERT-PRO X-ray diffractometer with $\text{CuK}\alpha$ irradiation ($k = 1.54059 \text{ \AA}^\circ$) and operated at 40 kV and 100 mA. The surface morphology of the thin film was studied by scanning electron microscopy (ZEISS EVO Series Scanning Electron Microscope Model EVO18).

3. Result and discussion

3.1 Structural analysis

X-ray diffraction technique was used for the structural analysis of CdO thin films. Fig.3 shows the X-ray diffraction plot of the samples of CdO thin films. All the observed peaks fit well with

the polycrystalline face-centered cubic CdO crystal structure (ICSD#: 061554). The XRD spectra illustrate the peak corresponding to (111) and (200) lattice planes of the zinc blend structure. Moreover, no impurity peaks were noticeable in diffractograms within the sensitivity of XRD. The Interplanar Spacing was calculated by Bragg's equation [15]:

$$2d \sin \theta = n\lambda \quad (1)$$

where d is interplanar spacing, h is Bragg's angle, n is the order of spectrum, and λ is the wavelength of the X-ray used. The lattice constant has been evaluated using the equation [16]:

$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}} \quad (2)$$

where h ; k ; l is the Miller indices. The calculated interplanar spacing and lattice constant values are shown in Table 1. The volume of the unit cell was also calculated. The variation of peak position (2θ), FWHM, d-spacing values, lattice parameters, and volume of the cell are listed in Table 1. The crystallite size of nanocrystalline thin films was estimated from the full width at half maximum (FWHM) from the strongest peak (111) plane using basic Scherrer's equation [17] and is tabulated in Table 1:

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (3)$$

where D is the average crystallite size, λ is the X-ray wavelength, β is FWHM (full-width half maxima), θ is Bragg's angle and k is the so-called Scherrer constant. k depends on the crystallite shape and size distribution, indices of the diffraction line, and the actual definition used for β whether FWHM or integral breadth [18]. k can have values anywhere from 0.62 to 2.08. In this paper $k = 0.9$ was used. In this work, the calculated values of D represent estimates [19]. The average crystallite size of the CdO films slightly decreased with an increase in concentration. The values of the crystallite size of the films were found to be in the range of 14-15 nm. The decrease in size results in an increase in the defects in the deposited thin films.

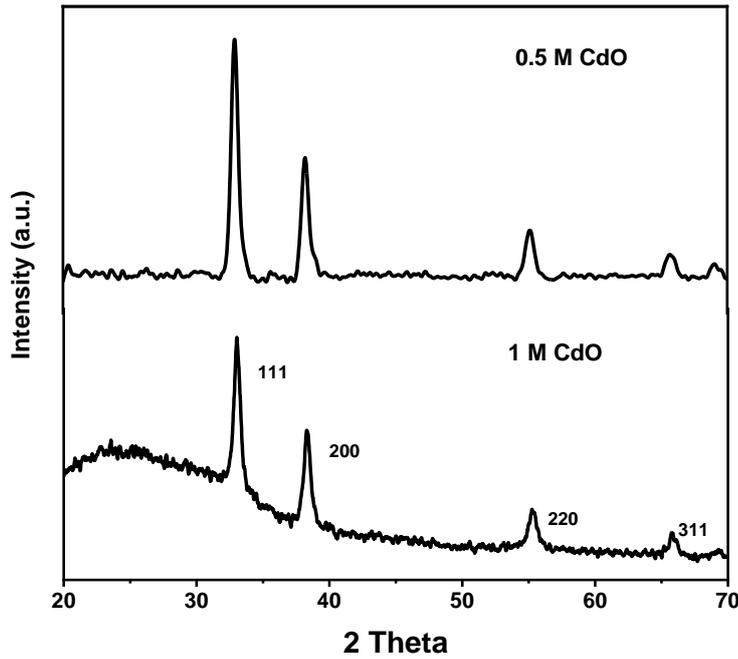


Fig. 1 XRD patterns of 1 M and 0.5 M CdO thin films.

Table 1 Values of 2θ and hkl , crystallite size (D), d-spacing lattice constant (a), volume of unit cell of Ho-doped CdO thin films

Samples	2θ	hkl	FWHM (β)(Theta)	Crystallite Size (D) (nm)	d-spacing (\AA)	Lattice constant (a) \AA	Volume of unit cell
1 M CdO	33.04	(111)	0.53	15	2.71	4.70	103.45
0.5 M CdO	32.92	(111)	0.55	14	2.72	4.70	104.55

3.2 Optical properties

Fig.2 shows the optical transmittance spectra of spin-coated CdO thin films as a different concentration. It is observed that all the deposited films exhibit a high transmittance in the wavelength range of 400-1100 nm. In comparison with 1 M CdO, 0.5 M CdO films have higher transmittance. Fig.3 shows the optical absorbance spectra of CdO thin film deposited by spin coating. All films have a uniform pattern of absorption. They show lower absorption in the higher wavelength region. There is a decrease in the absorbance of films with increasing concentration. After a comparison of absorbance and transmittance of different rates of CdO thin films. The optical bandgap was evaluated by the Tauc method; the optical absorbance region was defined according to the following equation [20]

$$(\alpha h\nu)^{\frac{1}{n}} = A(h\nu - E_g) \quad (4)$$

where A is a proportionality constant, E_g is bandgap and n is the constant which designates the type of transition. The blue shift of the absorption edge can be explained by the Moss–Burstein (M–B) effect [21]. The direct-allowed optical band gap was estimated by extrapolating the linear portion of $(\alpha h\nu)^2$ Vs $(h\nu)$ plot to the x-axis (Fig. 4). As the graph is linear, the transition is a direct transition and its value is taken as $\frac{1}{2}$ for an allowed direct transition. The intercept

on the x-axis (at $y = 0$) gives the directly allowed optical band gap. Calculated E_g values are in the range of 2.1 -3.06 eV as given in Fig.4 depending on the concentration of CdO thin films. It is noticed that the band gap of CdO initially increased from 3.06 eV (which is comparatively lower than the bandgap of the bulk CdO (2.1 eV)) and 0.5 M CdO thin film band gap of 2.1 eV. This change in the optical band gap values of the film can be the result of the change in the crystal structure of the CdO films as a result at different rates. The change in the crystal structure of the CdO films is a result of different rates. The change in the crystallite size of the films mentioned in the structural analysis part directly affects the optical properties of the materials.

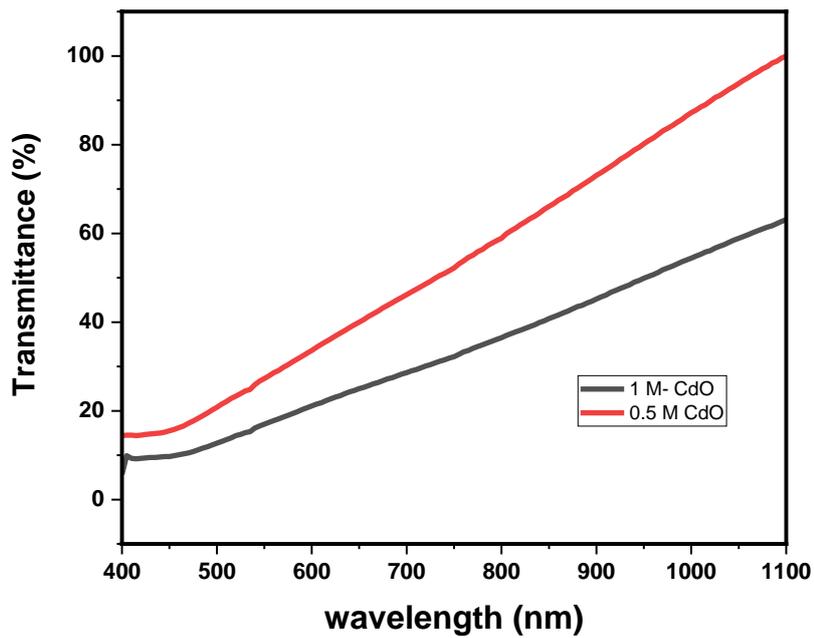


Fig. 2 Transmittance spectra of the CdO thin films.

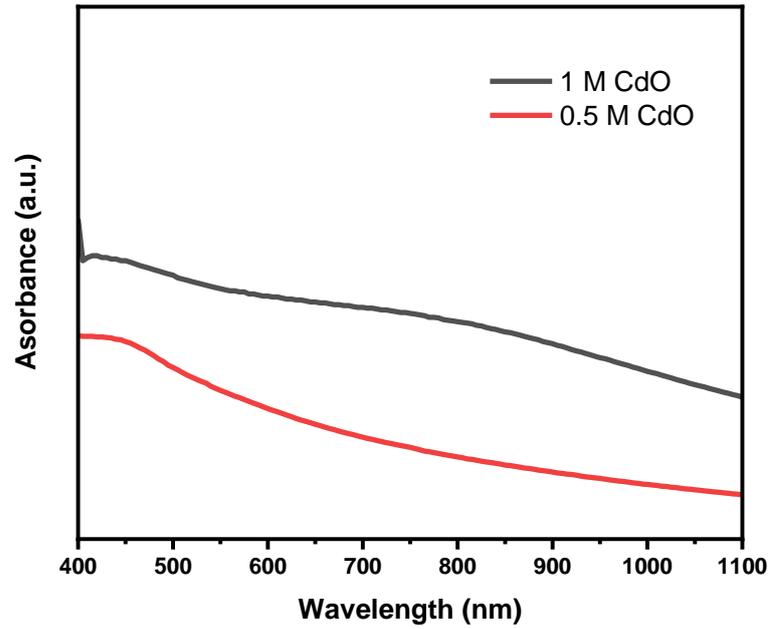


Fig. 3 Absorbance spectra of the CdO thin films.

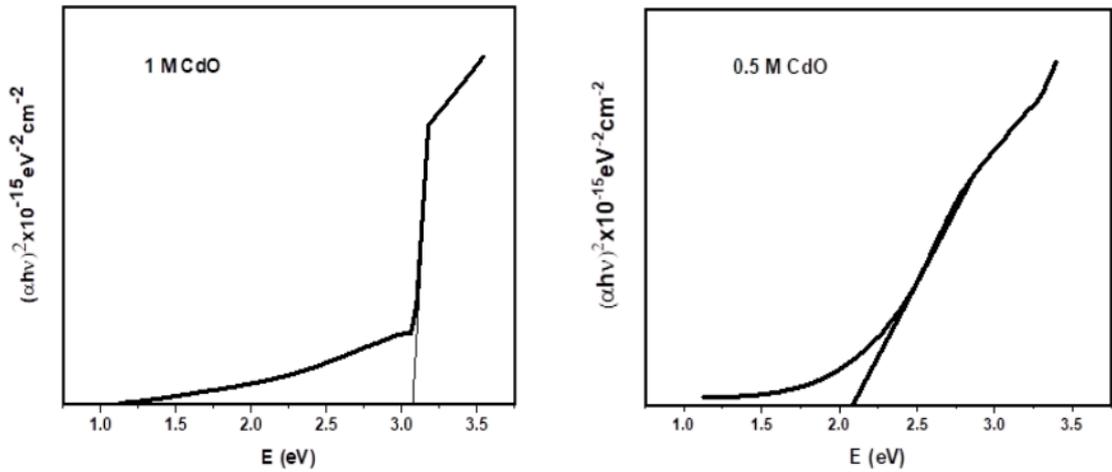


Fig. 4 Optical Band gap variation of the CdO thin films.

The extinction coefficient computes the amount of light loss owing to scattering and absorption per unit volume of penetrating medium. The extinction coefficient (k) was evaluated by using equation [22]

$$k = \frac{\lambda \alpha}{4\pi} \quad (5)$$

where α is the absorption coefficient and λ is the wavelength. It has the highest value for 0.5 M CdO thin films at a lower wavelength and its value decreases with increasing concentration.

The extinction coefficient decreases gradually with an increase in wavelength. This verifies that with increasing wavelength there is a decrease in loss of light by scattering as well as by absorbance.

The refractive index of deposited films gives knowledge such as film density, cavities in the film, speed of light in the films, etc. It was evaluated by the Herve– Vandamme formula [23]

$$n^2 = 1 + \left(\frac{A}{E_g + B} \right)^2 \quad (6)$$

where A and B are constants having values of 13.6 eV and 3.4 eV. The refractive index was found to increase from 2.33 to 2.66 for all the deposited films. Refractive index changes also account for crystallite size and internal strain of the film.

4. Conclusion

Various concentrations of CdO thin films were studied for their optical and structural characteristics. The sol-gel spin coating technique was used to successfully deposit the CdO thin films on a suitably clean glass substrate. It was found that every sample in the present investigation exhibited a cubic-type structure and was orientated along the (111) direction. The XRD studies also reveal that the deposited films have an average crystalline size in the range of 15-14 nm. The optical studies show the 0.5 M CdO thin film optical band gap is 2.1 eV. The extinction coefficient and refractive index also vary for different rates of CdO thin films. Thus, all the above properties reveal that these films are appropriate for different optoelectronic applications.

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6. References

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