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Structural and optical properties of chemically sprayed CuO thin films

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Spray pyrolysis deposition of CuO thin films using different concentration of aqueous solution containing $CuCl_2.2H_2O$ and double distilled water. The X-ray diffraction and transmission spectra of such films are recorded. X-ray diffraction patterns show that the films are polycrystalline and monoclinic in structure. The optical band gaps (1.45 to 1.76eV) are also determined from the optical transmission spectra.

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Keywords :Copper oxide thin film, Spray pyrolysis, UV-VIS-NIR spectroscopy XRD

1. Introduction

Copper oxide is a p-type semiconductor used as a passive component and also as an active one in solar cell technology and photovoltaic applications [1-5]. Moreover CuO is considered as a material in a capacitive type gas sensor for sensing and detecting a large number of gases [6]. Thin films of copper oxide have been prepared using various thin films deposition technique such as chemical vapour deposition, electro-deposition, thermal oxidation and sputtering process [7-9]. The present investigation deals with the study of CuO film prepared by spray pyrolysis. The films have been characterized for structural and optical properties using XRD and spectrophotometry, respectively.

2. Experimental technique

CuO thin films were deposited on conduction glass substrate by spraying with different concentration of(0.05M, 0.1M and 0.15M) aqueous solution of $CuCl_2 2H_2O$ dissolved in double distilled water. The experimental conditions of the spay deposition of films have been summarized in Table 1:

Table 1. Conditions for the deposition of CuO films.

Spray parameter	Values
$CuCl_2 2H_2O$	0.05M to 0.15M
Solvent	Double distilled water
Substrate temperature	400°C
Carrier Gas	Compressed air
Rate of Spray	4ml / m
Angular distance	25cm

The basic reaction involved in the film formation as,

$$CuCl_2 + H_2O \longrightarrow CuO + 2HCl$$

3. Results and discussion

3.1 Structural characterization

Structural characterization of films was carried out by XRD, employing X-Ray diffractometer (BRUKEL AX S D8), using Cu-Kα wavelength. Fig.1 to Fig. 3 show the X-ray diffraction patterns of film deposited at various mole concentration of aqueous solution The presence of sharp peaks are shown in all diffractograms and reveals that the sprayed CuO thin films are polycrystalline in nature. Results of peak positions observed for the films prepared at three different molar concentrations are compared with ASTM data. The preferred orientation is (111) crystal plane for all composition. The Copper Oxide thin films of different mole concentration are found to exhibit monoclinic in nature [10].

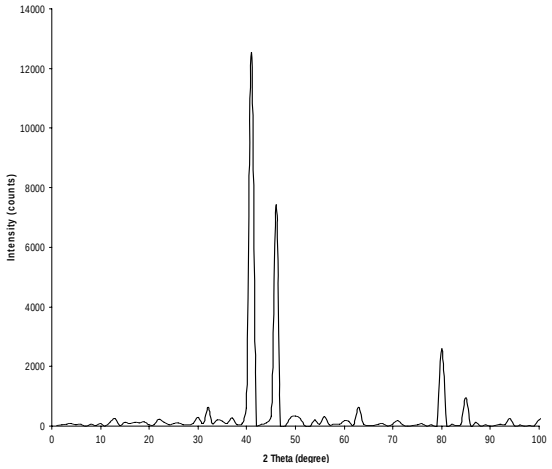

Fig. 1. Shows the X-ray diffraction pattern of CuO at 0.05 mol-concentration.

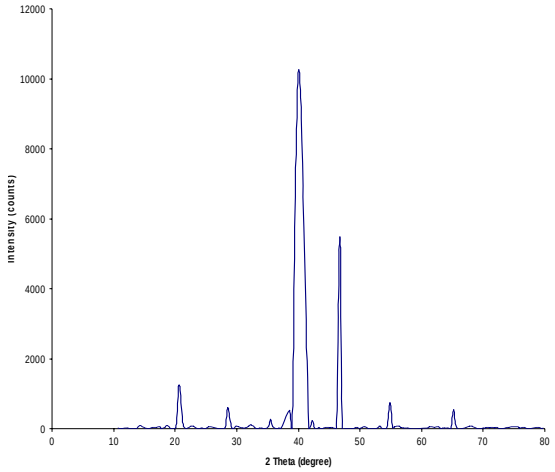

Fig. 2. Shows the X-ray diffraction pattern of CuO at 0.1 mol.

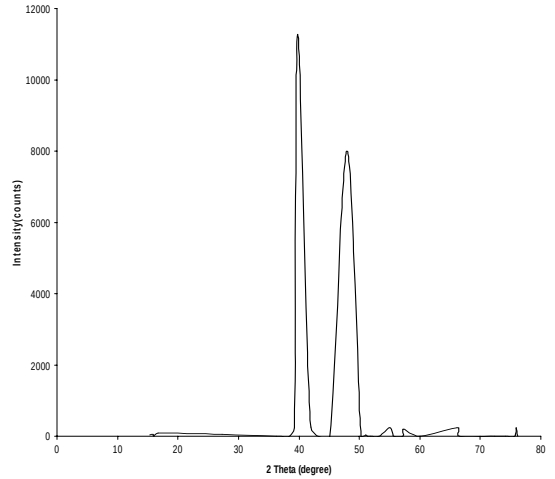

Fig. 3. Shows the X-ray diffraction pattern of CuO at 0.15 mol.

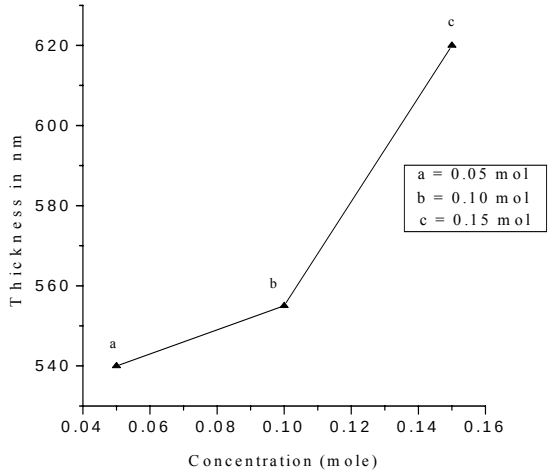

Fig. 4. Variations of film thickness Vs concentration of CuO thin film.

The Fig. 4 shows the variation of film thickness with respect to mole concentration of CuO sprayed thin films. It shows that the thickness of the film increases with increasing mole concentration of aqueous solution of copper chloride

3.2 Optical properties

The optical transmittance(%T) of sprayed CuO thin films were measured at room temperature using UV-VIS-NIR (VARIA CARRY-5000) Spectrometer. The transmission was recorded in the range of 300 nm to 1600 nm of the incident beam.

The variation of optical density with wavelength was analyzed to find out the nature of transition involved and the optical band gap, using the relation "[11]"

$$\alpha = \frac{A(h\upsilon - E_g)}{h\upsilon}$$

where, A is a constant and E_g is the band-gap energy.

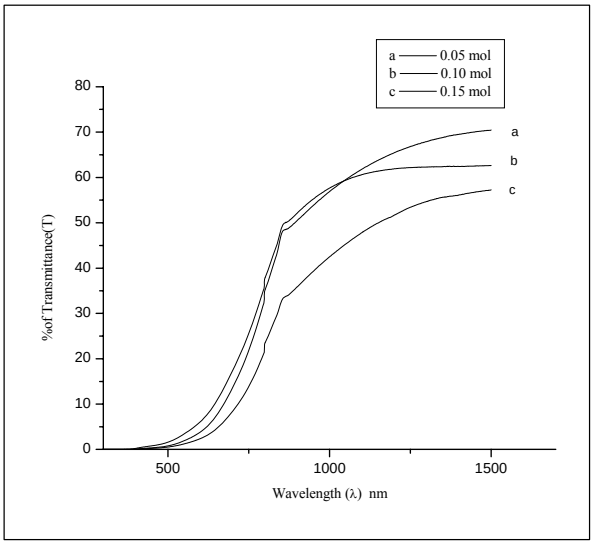

Fig. 5. Optical transmittance spectra of CuO.

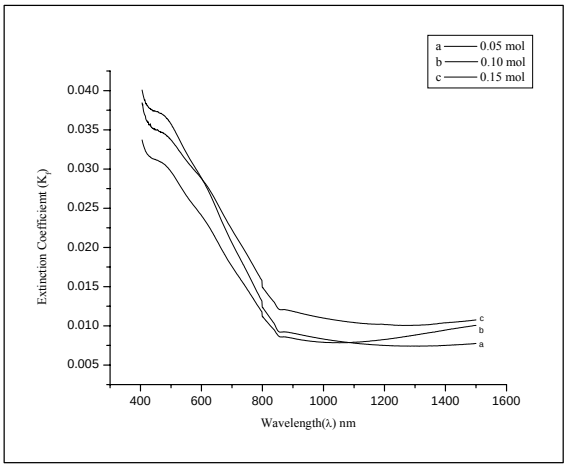

Fig. 6. Extinction coefficient CuO.

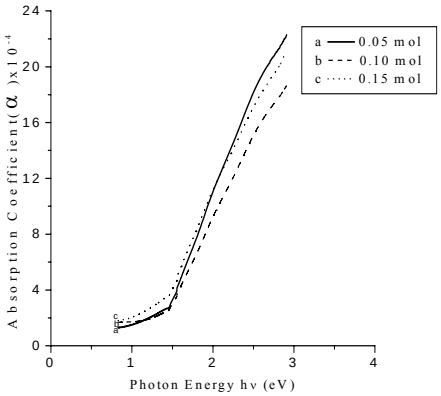

Fig. 7. Variation of absorption coefficient (α) with photon energy (hν) of CuO thin films.

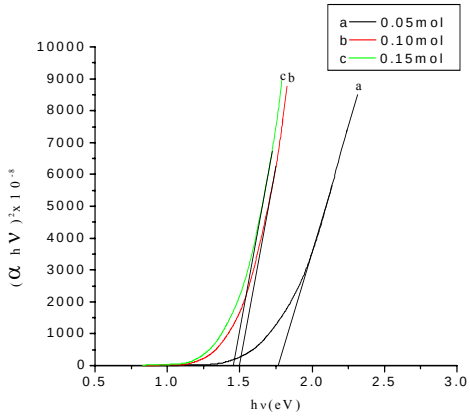

Fig. 8. Variation of $(\alpha h\nu)^2$ as the incident photon energy (hν) of CuO films at different molar concentrations.

Fig. 5 shows the optical transmittance spectra of CuO with the wavelength. The percentage of transmittance value (%T) in the visible region is found to increase with decreasing mole concentration of the solution. The maximum transmission behavior is observed for lower mole concentration and comparatively lower values are recorded for other concentrations. This is attributed to the increase of the film thickness with increasing mole concentration of the films.

From the optical data the extinction co-efficient (K_f) and absorption co-efficient(α) are measured. Fig. 6 shows the variation of extinction co-efficient with the wavelength. It shows that it decreases with increasing wavelength.

The absorption co-efficient is minimum at lower energy and increases with increasing optical energy. It also shows the linear variation at the absorption edge. It reveals that the optical transition of the film is direct allowed transition [12].

Fig. 8 shows the variation of $(\alpha h\nu)^2$ as the incident photon energy (hν) of CuO films at different molar concentrations. When the linear portion of the graph is exactly plotted the intercept of X - axis gives the band gap values of those films.

Table 2. Optical parameters.

Concentration (mol)	Transmittance (% T)	Band gap energy (eV)
0.05	70.4661	1.76
0.10	62.6410	1.50
0.15	57.24448	1.45

Table 2 shows the values of band gap energy of the film with different concentrations of CuO. It reveals that the energy gap of Copper Oxide films increases with decreasing mole concentration of $CuCl_2$. The variation of band gap of CuO films is between 1.45 and 1.76 eV. This range the suitable to use the material for solar cell application

4. Conclusions

Copper oxide thin films have been prepared by chemically spraying of aqueous solution of copper chloride and their deposition conditions are optimized. The films are polycrystalline in nature. The texture of the films are found to be in (111) plane. The structure of the films is monoclinic. The molar concentration of the films affects the thickness and optical properties of the films. The transmittance increases with decrease in concentration of the films. The optical band gap was also found to vary from 1.45 to 1.76 eV. Hence CuO thin films are suitable for solar cell applications.

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