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Structural properties of Cd-doped copper oxide thin films on Glass substrate prepared by Spray Pyrolysis technique

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Abstract: Cd doped CuO thin films are prepared onto the glass substrate. Thin films pure and Cd doped CuO are deposited by spray pyrolysis. CuO is a n-type semiconductor with indirect band gap which was suitable for solar cell applications. The structural properties of thin films were investigated using XRD patterns. The X-ray diffraction patterns confirm the deposited thin films have monoclinic crystal structure. The structural properties such as lattice constants and volume of unit cell are calculated and discussed. The crystallite size was calculated using Scherrer's equation and found to be in the range of 5-7 nm. The values of microstrain increased slightly for Cd doping in CuO thin film.

Keywords:Copper oxide; Cd doping; thin films; X-ray diffraction, micr-strain.

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I. INTRODUCTION

Transition metal oxides materials have great interest recently due to their potential applications such as solar cells, light emitting diodes, optoelectronics and gas sensing [1-4]. Among them, Copper oxide (CuO) is a promising material due to single phase n-type semiconductors with anindirect band gap of 1.3–2.1 eV [5]. The CuO have monoclinic crystal structure. The applications of CuO were gas sensors, solar energy, diode fabrication, lithium ion batteries, electrochemical cells, superconductor, photovoltaic, nano-electronics and spintronics [5-9].

The copper oxide (CuO) has also been prepared by several routes, such as thermaloxidation [10], simple solution [11], simple hydrolysis [12], template-based sol–gel [13], and electrochemical [14].Besides, the hydrothermal [15-19], solvothermal [20, 21] and microwave-hydrothermal [22-23] methods have alsobeen employed to control the morphologies of these oxides. Compared with other deposition techniques, spray pyrolysis is especially efficient, due to its high deposition rate and low cost. In this paper, we report the synthesis and structural properties of Cd doped CuO thin films by a spray pyrolysis. The structural properties such as lattice parameters, volume, crystallite size, microstrain and dislocation densities are calculated and discussed. The effects of Cd doping on structural properties of the CuO thin films have been studied.

1. Experimental details

CuO thin films prepared on glass substrate using spray pyrolysis technique. The precursor used for CuO thin films is cadmium acetate. These precursors are dissolved in double distilled water separately having unique 0.1M concentration. A substrate temperature is constant at 350^0C. The other parameters kept constant. The spray nozzle to substrate distance is fixed 30cm. With suitable air pressure used as an carrier gas, solution can be sprayed on glass substrate by using spray machine. Well adherent and uniform films were deposited successfully. After deposition note spray rate and cool the substrates at room temperature for good crystallized films. First deposition is for pure and undoped film of CuO without any doping in it. Later on taking percentage of doping of Cd that is 1%, deposition is taken on glass substrate. Structural characterization of prepared samples was measurement using x-ray diffraction (Model: PW-3710). The structural analysis of the synthesized samples was carried out using a powder X-ray diffractometer (XPERT-PRO) with a Cu-Kα radiation source of wavelength 1.5406 A^0.

II. RESULTS & DISCUSSIONS

The XRD patterns of thin films for CuO and Cd doped CuO are shown in figure 1(a) and 1(b). The maximum diffraction peaks appeared at 2θ=35.50° and 38.61°corresponds to (002) and (111) planes of Monoclinic phase. The lattice parameters calculated using the XRD patterns, it was found that for pure CuO thin

films a= 4.7270Å, b=3.4269Å and c=5.1258Å and for 3% Cd doped CuO are a= 4.7222Å, b=3.4086Å and c= 5.1260Å. Form this result it was clear that the lattice parameters increase with increasing Cd doping. The volume of unit cell for pure CuO and Cd doped CuO films was 81.88 $(Å)^3$ and 81.33$(Å)^3$ respectively.

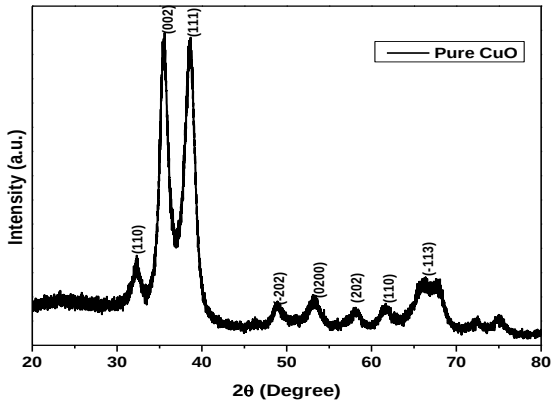

Figure 1(a). XRD patterns of pure CuO thin film.

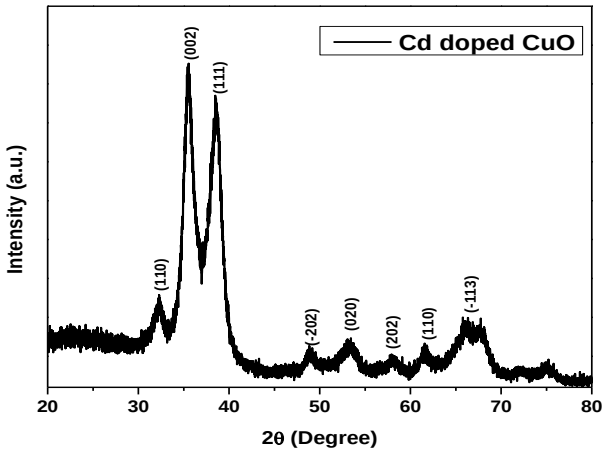

Figure 1(b). XRD patterns of Cd doped CuO thin film.

The average crystallite size was calculated using Scherrer's equation is given by

$$D = \frac{0.9\lambda}{\beta \cos\theta}$$

Where, D is crystallite size, λ is the X-ray wavelength (Cu Kα; 1.5405 Å), β is full width at half maximum (FWHM) in radians, θ is the Bragg´s angle in degrees, K is the correction factor and D is the crystallite size. The average crystallite size for pure CuO thin film is 6.53 nm and Cd doped CuO is 6.04 nm. The average crystallite size was decreased with increasing Cd content due to the small grain growth of pure CuO films as compared to the Cd doped CuO thin films. The micro-strain was determined using the following equation:

$$\varepsilon = \frac{\beta}{4\tan\theta}$$

Dislocation density is calculated using the expression [24]:

$$\delta = \frac{1}{D^2}$$

The micro-strain and dislocation density areincreased from 0.0181 to 0.0203 and 2.31×10^{14} to 2.74×10^{14} line/m^2 in Pure and Cd doped CuO thin films. The micro-strain and dislocation densities enhancement with Co doping, it may be due to the reduction of average crystallite size with Cd content.

III. CONCLUSION

In summary, highly (002) and (111) orientated pure and Cd doped CuO thin films have been prepared using spray pyrolysis. The XRD patterns indicate the crystalline of single phase of CuO in pure and Cd doped CuO thin films. Trace amount of Cd in thin films doesn't to the XRD peaks. The lattice parameters slightly increased with Cd doping. The crystallite size, micro-strain and dislocation density determined using XRD patterns. The micro-strain and dislocation density increased whereas average crystallite size decreased with increasing Cd doping.

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