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Research Paper

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Effect of molarity variation on band gap of CuO Nanostructures Synthesized by wet chemical method

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***Abstract*—** The wet chemical method has been implemented to synthesize CuO nanostructures at 100^0C. The monoclinic phase structure of CuO nanostructures has been affirmed by X-ray Diffraction (XRD) pattern. Crystal size and dislocation density of the nanostructures have been calculated from XRD data. UV-visible absorption spectra have been used to estimate band gap of the prepared CuO nanostructures. The refractive index and dielectric constant of CuO nanostructures have been calculated from band gap which shows an increase with the decrease of the band gap. Field Emission Scanning Electron Microscopy (FESEM) has been used to inspect the crystals' surface morphology.

Keywords—*Nanostructures, XRD, optical band gap, FESEM*

I. INTRODUCTION

Nanostructure properties diverge from bulk counter part due to their distinguishable electronic, optical and chemical aspects. Metal oxide nanostructures play an important role in nanotechnology. These nanostructures are extensively used in innumerable applications. Copper oxide (CuO) nanostructures is also one of that category metal oxide. CuO nanostructures are mostly utilized in numerous of applications such as solar cells, humidity sensor, gas sensor, photo catalyst, antimicrobial, organic dye remover, toxic element remover, heavy metal remover from water [1-15]. Numerous methods are used to synthesized CuO nanostructures such as chemical bath deposition, vapour deposition, microwave assist synthesis, hydrothermal synthesis, sol-gel, spray pyrolysis, solid state thermal decomposition [16-22]. The sol-gel method is one of the cost-effective methods for preparing CuO nanostructures. In this paper, we have prepared CuO nanostructures with the help of sol-gel method and analysed its different structural and optical features.

This paper has been organized into four portions - Introduction, Materials and Methods, Results and Discussion and Conclusion. Introduction portion gives a brief review of literature related to our present work. Materials and Method portion contains the materials used for the preparation of CuO nanostructures and details of preparation procedure of CuO nanostructures at different molarities by sol-gel method with special reference to characterization tools. Results and Discussion portion provides a brief detail on the characterizations of the CuO nanostructures and analysis and discussion of the results obtained. Conclusion portion provides major conclusions drawn from the results.

II. MATERIALS AND METHODS

All the required materials for synthesizing CuO nanostructures by the sol-gel method, such as $Cu(NO)_3.3H_2O$, NaOH and glacial acetic acid were bought from the market with the highest purity. The aqueous solution of $Cu(NO)_3.3H_2O$ (0.4M) was prepared in 50ml DI water dissolving the required amount of $Cu(NO)_3.3H_2O$ in a beaker. Dropwise addition of 1 ml of glacial acetic acid was done to the above solution with constant stirring and then heated to 100^oC.8.5 pH was maintained by dropwise addition of 8M NaOH solution to the above solution. A change in colour of the solution was observed and a black precipitate was formed. The precipitate was filtered and washed 4 times with deionized water. Then the precipitate was dried in air and converted into powder using mortar. The powders were used for further analysis and characterization of CuO nanostructures.

A similar method was applied to synthesized CuO nanostructures from 0.6M $Cu(NO)_3.3H_2O$ aqueous solution.

Structural characterization of prepared CuO nanostructures was done by XRD using Philips X'pert Diffractometer with CuKα radiation (λ=1.5406 Å). Carry 300 scan UV-Visible spectrophotometer was used to measure optical absorption

spectra. The morphology of prepared CuO nanostructures was studied by Field Emission Scanning electron microscope, ZEISS, SIGMA.

III. RESULTS AND DISCUSSION

A. Structural Analysis

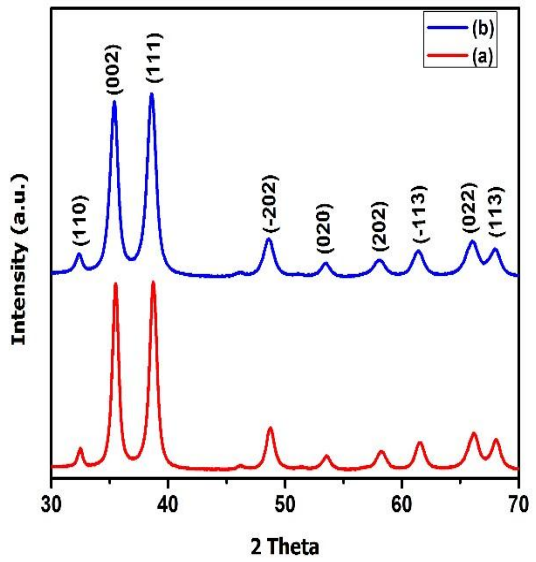


Fig 1: XRD pattern of CuO nanostructures prepaped at (a)0.4M,and (b) 0.6M

X-Ray Diffraction pattern is used for determining the structure and phase of prepared CuO nanostructures. Fig.1 shows the XRD diffraction pattern of prepared CuO nanostructures at different molarities (0.4M and 0.6M). The diffraction pattern exhibits clear peaks centred at various angles corresponds to (110), (002), (111), (-202), (020), (202), (-113), (022) and (113) planes as shown in Table1. All the peaks in the diffraction pattern show the prepared CuO nanostructures are of monocline structure. The peaks are matched with the standard data of ICDD card no. 89-5895. The Debye-Scherrer's equation is used to find the crystallite size (D) of prepared samples [23].

$$D = \frac{K\lambda}{\beta \cos\theta} \qquad (1)$$

Where K is a constant and equal to 0.9, λ = wavelength of X-ray radiation (λ=1.54056 Å for CuK_α radiation), β = FWHM (full width at half maximum, in radian) and θ =the Bragg's diffraction angle. The calculated values of crystallite size are given in Table 1.

The dislocation density of CuO nanostructures has been estimated by using the equation [24]

$$\text{Dislocation Density } (\delta) = 1/(D^2) \qquad (2)$$

Where D is the crystallite size. The calculated values of the dislocation density of the CuO nanostructure samples are given in Table 1.

Table1.Structural parameters of CuO nanostructures prepared at various molarity

Sample	Angle	hkl	Size obtained by Debye Scherrer formula	Dislocation Density
	($2\Theta^0$)		(nm)	($\delta x10^{16}$ m^{-2})
CuO nanostructure (0.4M)	32.51	(110)	20.15	0.00246
	35.5	(002)	12.86	0.00605
	38.74	(111)	10.59	0.00892
	48.75	(-202)	9.09	0.01210
	53.51	(020)	7.1	0.01984
	58.24	(202)	6.94	0.02076
	61.55	(-113)	8.29	0.01455
	66.12	(022)	7.38	0.01836
	68.06	(113)	9.17	0.01189
CuO nanostructure (0.6M)	32.38	(110)	13.12	0.00581
	35.35	(002)	10.07	0.00986
	38.59	(111)	9.26	0.01166
	48.6	(-202)	11.6	0.00743
	53.44	(020)	28.43	0.00124
	58.09	(202)	15.77	0.00402
	61.54	(-113)	20.67	0.00234
	66.08	(022)	8.94	0.01251
	68.06	(113)	19.85	0.00254

B. Optical Absorption Analysis

Different optical properties of the prepared CuO nanostructures were studied by recording optical absorbance spectra in the range 200-800nm. The information of optical absorbance and band gap energy of a material predicts the area in which it can be used.

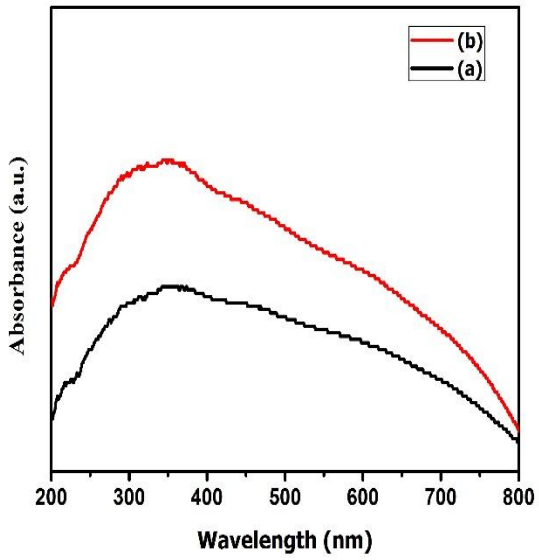


Fig 2. Absorption spectra of CuO nanostructures prepared at (a)0.4M and (b)0.6M

The Fig 2. shows optical absorption spectra of CuO nanostructures synthesized at different molarities (0.4M and 0.6M) [25-26].

The optical band gap energy (E_g) is calculated by using Tauc's formula [27]

$$(\alpha h\nu)^{1/n} = A(h\nu - Eg) \qquad (3)$$

Where α is the absorption co-efficient, $h\nu$ is the incident photon energy, A is a constant. For direct band gap material, n=1/2. The band gap energy has been estimated by plotting graph $(\alpha h\nu)^2$ versus $h\nu$ and then extrapolating the linear region of plots as shown in Fig 3. The band gap energy of CuO nanostructures prepared at 0.4M and 0.6M are estimated as 1.82 and 1.71 eV respectively.

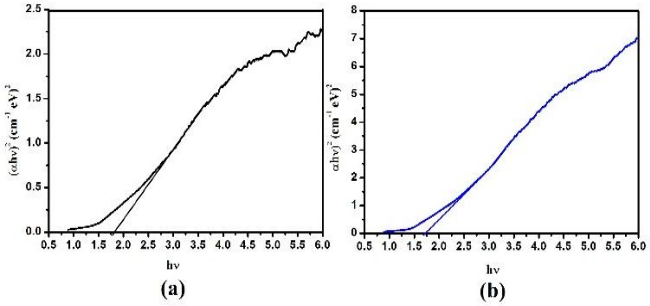


Fig 3. $(\alpha h\nu)^2$ vs $h\nu$ spectra of CuO nanostructures prepared at (a) 0.4M and (b) 0.6M

Refractive index for prepared samples are estimated with the help of Herve and Vandamme relation [28]

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2} \qquad (4)$$

Where A=13.4 eV and B=3.4 are constants. This relation is applicable to the materials having high band gap energy. The estimated value of refractive index is shown in Table 2.

Optical dielectric constant (ε_α) is evaluated from the relation [29]

$$\varepsilon_\alpha = n^2 \qquad (5)$$

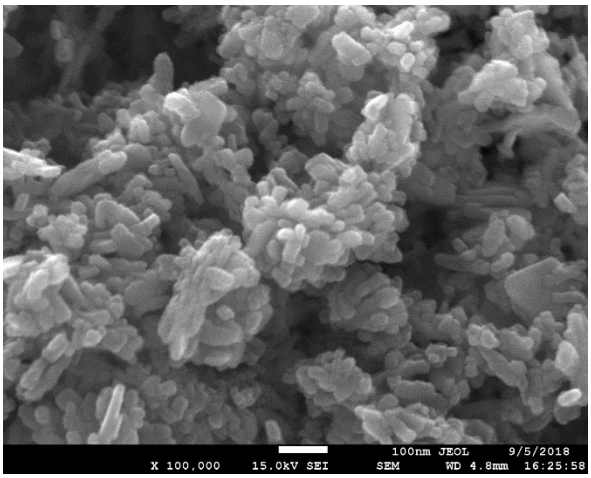
Where n is representing the refractive index. The calculated value of dielectric constant is given in Table2.

Table 2: Optical parameters of prepared CuO nanostructures

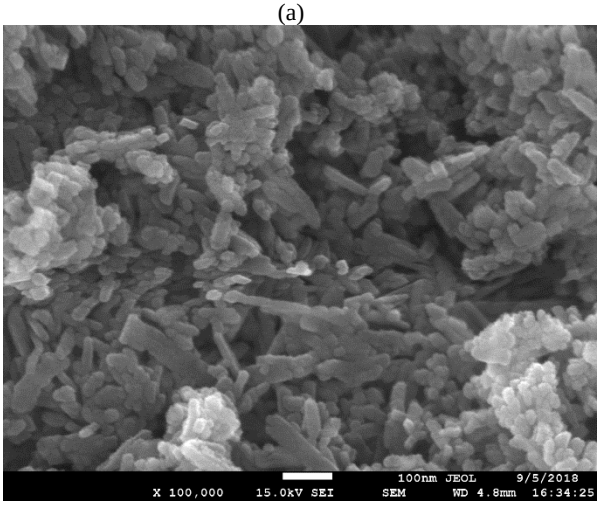
Sample	Band gap, E_g (eV)	Refractive index	Dielectric constant (ε_α)
CuO nanostructure(0.4M)	1.82	2.754949132	7.589744719
CuO nanostructure(0.6M)	1.71	2.806511273	7.876505528

C. FESEM Analysis

The surface morphology and micro structure of prepared CuO nanostructures were investigated with the help of FESEM images as shown in figure 4. It clearly shows the almost rod shape morphology of prepared CuO nanostructures with an uneven distribution. Agglomeration of rod shape CuO nanostructures was also observed from the FESEM images.



(a)



(b)

Fig 4. FESEM images of CuO nanostructures prepared at (a)0.4M, and (b) 0.6M molar concentration of precursors

IV. CONCLUSION AND FUTURE SCOPE

Copper oxide nanostructures are successfully prepared by sol-gel method. XRD pattern shows the prepared nanostructures are of the monoclinic structure. It is observed that with the increase of crystallite size, the dislocation density decreases. With the increase in molarity of precursors, the band gap of prepared nanostructures decreases. When the band gap decreases, refractive index and dielectric constant increases. FESEM images show the morphology of prepared CuO nanostructures. We plan to investigate the antibacterial activity of prepared CuO nanostructures as our future work.

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