

XRD and Band Gap Study of SrDopedCuONano Particles by Sol Gel Method

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ABSTRACT

In this work Strontium doped copper oxide nanoparticles were prepared by sol gel method. Different samples were prepared by changing the concentration of Strontium . Prepared samples were studied using X ray diffraction and analysis shows that particles size increases with increase in strontium concentration from 34.7nm to 89.9nm. UV-VIS spectroscopy shows that band gap decrease with increase in strontium concentration from 5.39 eV to 5.10 eV.

Keywords : Nanomaterials, XRD, UV-VIS, Band Gap, Doped Metal Oxide

I. INTRODUCTION

Nanomaterials are different from bulk materials because of their chemical, optical and electronic properties [1, 2]. They show extremely fascinating and useful properties, which can be exploited for a variety of structural and non-structural applications [3]. Metal oxide nanoparticles belong to a family of nanomaterials that have been manufactured on a large scale for both industrial and household applications and they hold promise for future applications [4, 5]. Copper Oxide is an extensively studied group II-VI semiconductor with optical properties that permits stable emission at room temperature having immense application in sensors, field emission and photonic devices [6]. Nanoparticles of CuO can be used as gas sensors, optical switch, and magnetic storage media owing to its photoconductive and photochemical properties [7]. Furthermore it is a promising semiconductor for solar cell fabrication due to its suitable optical properties. CuO nanoparticles have immense medical applications [8- 10]. It possesses useful photovoltaic and photoconductive properties because CuO crystal structures have a narrow band gap [11, 12]. CuO nanoparticles have been applied in different areas, including sensors catalysis, batteries, high temperature superconductors, solar energy conversion, and field emission. In the present study we have synthesized strontium doped copper oxide nanoparticles by sol-gel method by taking different concentration of strontium .

II. METHODS AND MATERIAL

All the reagents used were of analytical grade.. Strontium Nitrate [Sr(NO₃)₂], Copper Nitrate Cu(NO₃)₂ .3H₂O and Ethanol (CH₃CH₂OH) were used as raw Materials and poly vinyl alcohol (PVA) as the sol-gel forming solvent. For synthesis of Sr_{0.1}Cu_{0.9}O, we take 2.1163 g of Sr(NO₃)₂ and 21.744 g of Cu(NO₃)₂ .3H₂O . We mix 50 ml of distilled water in 50 ml of ethanol and then add these two nitrates in this solution with constant stirring. Then we add 5g of PVA in this mixture. This mixture was then heated at 80°C with magnetic stirrer. After some time of heating a gel starts to appear. The solution is heated till whole solution is converted in to gel. Then this gel is dried for 24 hrs and then crushed and calcinated at 400°C. The fine powder is taken out for characterization. (13) Similarly we prepared other samples by varying concentration of strontium nitrate and copper nitrate

2.1 XRD ANALYSIS:-

The typical XRD pattern of nanoparticles of Sr_{0.1}Cu_{0.9}O, Sr_{0.3}Cu_{0.7}O, Sr_{0.5}Cu_{0.5}O, Sr_{0.7}Cu_{0.3}O

and Sr_{0.9}Cu_{0.1}O annealed at 400°C is shown in Figure 1. The peak positions of the sample exhibits the monoclinic structure of CuO which was confirmed from the ICDD card No 801916. Further, no other impurity peak was observed in the XRD pattern, showing the single phase sample formation. The crystalline size was calculated using the Scherer formula,

$$D = 0.9 \lambda / \beta \cos\theta \text{-----(1)}$$

where λ is the wavelength of X-ray radiation, β is the full width at half maximum (FWHM) of the peaks at the diffracting angle θ . Crystallite size calculated by the Scherer formula of each sample was shown in table.

Table of comparison of various XRD parameters

Name of sample	2 θ	D(nm)	FWHM	Relative intensity	Particle size(nm)
Sr _{0.1} Cu _{0.9} O	35.540	2.5239	0.251	100.00%	34.7
	38.715	2.3239	0.256	94.72	34.3
Sr _{0.3} Cu _{0.7} O	38.712	0.23241	0.254	100%	34.5
	35.884	0.25208	0.250	75.88%	34.9
Sr _{0.5} Cu _{0.5} O	25.159	0.35367	0.139	100%	61
	25.783	0.34525	0.130	54.27%	65.4
Sr _{0.7} Cu _{0.3} O	25.228	0.35272	0.116	100%	73
	25.863	0.34420	0.108	49.10%	78.6
Sr _{0.9} Cu _{0.1} O	25.177	0.35343	0.095	100%	89.9
	25.818	0.34480	0.095	47.79%	89.9

2.2 UV -VIS Analysis:-

The optical absorption spectrum was used to study the optical properties of the Synthesized nanoparticles. From this study we can determine the band gap and the type of electronic transitions. When a semiconductor absorbs photons of energy larger than the gap of the Semiconductor, an electron is transferred from the valence band to the conduction band and there occurs an abrupt increase in the absorbency of the material to the wavelength corresponding to the band gap energy. The relation of the absorption coefficient (A) to the incidental photon energy depends on the type of electronic transitions. When in this transition, the electron momentum is conserved, the transition is direct, but in an indirect transition if the momentum does not conserve. Band gap studies of these materials have been reported using absorption spectra. The fig.(2)

depicts the optical absorption spectrum of of Sr_{0.1}Cu_{0.9}O, Sr_{0.3}Cu_{0.7}O, Sr_{0.5}Cu_{0.5}O, Sr_{0.7}Cu_{0.3}O and Sr_{0.9}Cu_{0.1}O.

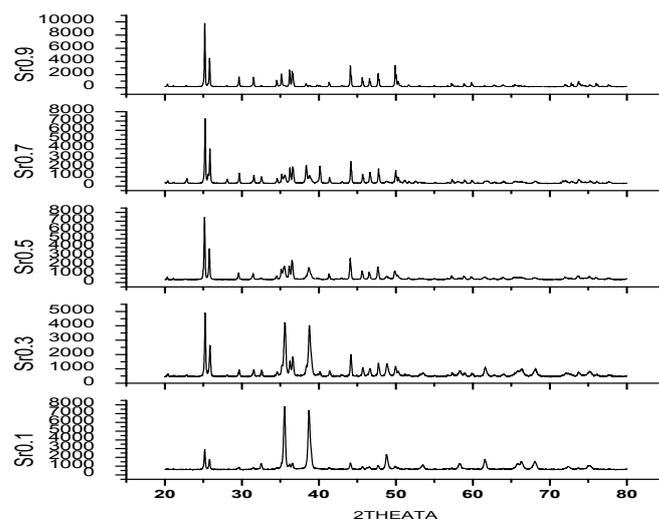


Figure 1. Comparative Analysis of XRD of all Five Samples

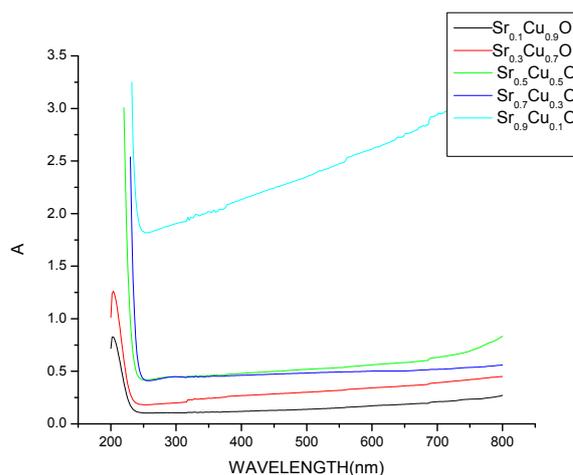


Figure 2

2.3 Calculation of Eg and particle size:-

The optical band gaps could be roughly estimated by empirical formula

$$(\alpha h\nu)^2 = A(h\nu - E_g) \text{-----(1)}$$

Where A is a constant that depends on the transition probability, Eg is the optical band gap energy, h is the Plank constant and ν is the frequency. The Eg was calculated by extrapolating a straight line to the $(\alpha h\nu)^2 = 0$ axis in the plots of the $(\alpha h\nu)^2$ versus optical band gap energy. In this way, the optical band gaps of samples were determined. Assuming that the transition

probability was 1, the equation could be simplified as listed below.

$$(\alpha h\nu)^2 = h\nu - E_g \text{-----(2)}$$

$$h\nu = hc/\lambda = 1240/\lambda \text{-----(3)}$$

Using equation(3) the equation (2) could be translated into the equation (4) listed below.

$$(\alpha 1240/\lambda)^2 = 1240/\lambda - E_g \text{-----(4)}$$

In the equation (3), α is the absorption value in the UV-VIS spectrum that could be detected by UV-VIS spectrophotometer, while λ is the detection wavelength. For example, figure (2) shows the UV-vis spectrum of all samples. According to the equation (3), figure(3) was achieved by treating $(\alpha h\nu)^2$ as Y axis and $h\nu$ as X axis. The E_g (eV) could be estimated by extrapolating a straight line to the $(\alpha h\nu)^2 = 0$ axis in the plots of the $(\alpha h\nu)^2$ versus optical band gap energy.

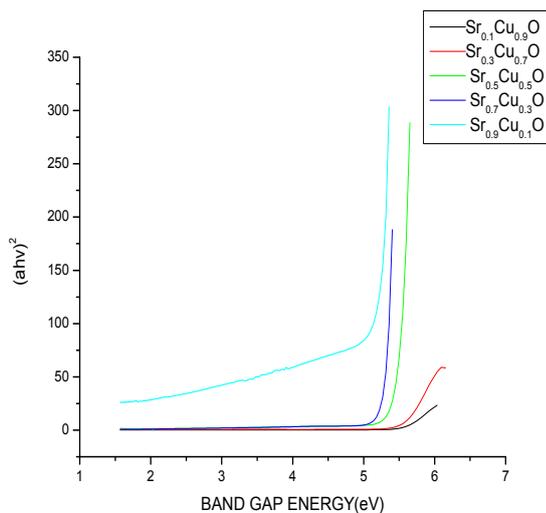


Figure 3.

And the the fig(4) shows the comparative value of band gap energy of all samples.

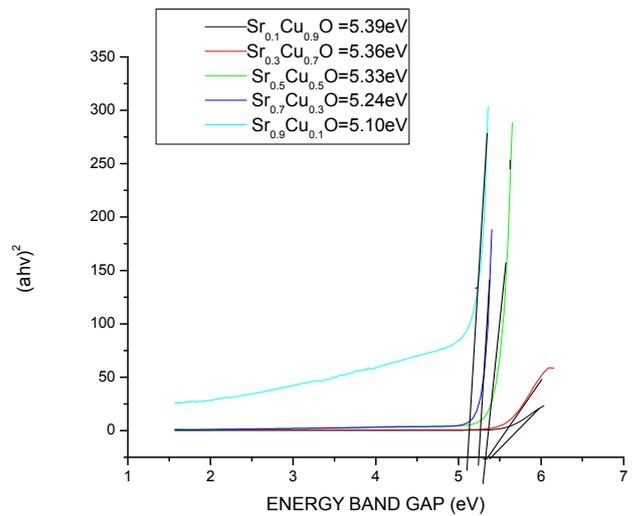


Figure 4.

Table for band gap energy of all samples

S.N.	NAME OF SAMPLE	BAND GAP ENERGY (eV)
1	Sr_{0.1}Cu_{0.9}O	5.39
2	Sr_{0.3}Cu_{0.7}O	5.36
3	Sr_{0.5}Cu_{0.5}O	5.33
4	Sr_{0.7}Cu_{0.3}O	5.24
5	Sr_{0.9}Cu_{0.1}O	5.10

So from UV-VIS analysis we see that as we increase the concentration of strontium ,band gap decreases.Fig (5) depicts it in graphical way

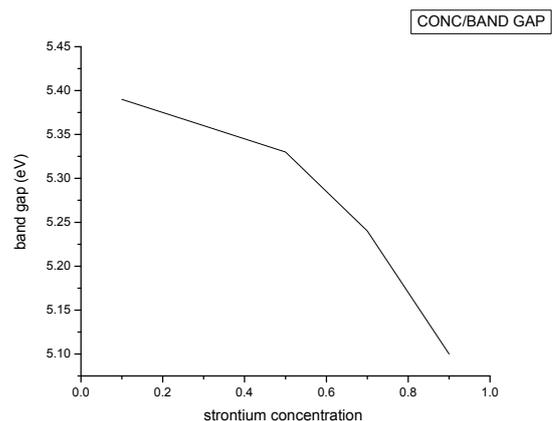


Figure 5.

III. RESULTS AND DISCUSSION

1. With increasing the doping concentration of Sr we see that relative intensity of copper peak which lies

- around 35 degree decreases while that of Sr peak which lies around 25 degree increases
- FWHM also goes on decreasing with increasing concentration of Sr.
 - Particle size goes on increasing with increasing concentration of Sr.
 - Band gap decreases with increase in Sr concentration.

IV. CONCLUSION

We see that as we increase the concentration of strontium, the size of nanoparticles increase which is obvious as radius of strontium atom are bigger than copper atom. We conclude band gap energy decreases with increase in strontium concentration. We also conclude that sol gel method is a very nice and simple method to prepare these nanoparticles which are all crystalline in nature as obvious from xrd samples.

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