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ORIGINAL ARTICLE **OPEN ACCESS**

Effect of Doping in Copper Oxide Nanoparticles Studied by X-Ray Diffraction

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ABSTRACT
CuO2 nanoparticle was prepared by applying computational method. Characterize the nanoparticle by operating XRD, SEM, and FTIR. X-ray diffraction is used to determine the exact grain size and crystal arrangement of the materials and used to verify doping exists, (101), (200) the hkl value proves doping exists in the prepared material. Scanning electron microscopy is suited to identify the size and morphology of the particles. After doping with the metal exhibit the cubic strictures and size below 100 nm. FTIR is used to identify the functional group (CHEM S- 2) that exposes the metal functional group of the nanoparticles. The present study defines the magnetic nature of CuO2 by using magnetic (Daniel B.Litvin) symmetry which is known by XRD and crystal impact Match-2 and Diamond-3 software. symmetric calculation spins aligned within the found to be little ferromagnetic. From the overall report, we get concluded that doping changes the magnetic nature of the CuO2 nanoparticle by changing its crystal structure and magnetic symmetry.

Keywords: CuO, XRD,SEM, and FTIR.

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INTRODUCTION

The oxides of transition metals are an essential class of semiconductors, which have applications in magnetic storage media, solar energy transformation, electronics and catalysis [1-9]. Copper oxides have extensively importance due to their unique properties which can enhanced or determined by synthetic processes. CuO employ exceedingly applications in superconductors, steam reforming, antimicrobial, humidity sensor, optical, catalysts for the water-gas shift reaction, and electrical technological6. [10-15].Copper oxides can either be Cu2O or CuO and both of them p-type with a narrow band gap of about (1.2 up to 1.4 eV) at room temperature [16-24].CuO synthesis based technique, hydrothermal, microwave and ultrasonic which have been enhanced to fabricate well-defined nanostructures with different morphologies. The size, shape and morphology of the CuO nanostructures are highly significance by different parameters such as concentration of constituents, temperature and aging time [25-28] However, the reports on the preparation and characterization of nanocrystalline CuO are relatively few to some other transition metal oxides such as zinc oxide, titanium dioxide, tin dioxide and iron oxide. Some methods for the preparation of nanocrystalline CuO have been reported recently such as the sonochemical method [29], sol–gel technique [30],one-step solid state reaction method at room temperature [31], electrochemical method [32],thermal decomposition of precursors [33] and co-implantation of metal and oxygen ions and so on.

MATERIAL AND METHODS

PREPARATION OF PURE COPPER OXIDE NANOPARTICLES

Copper borate (1.0) mole dissolved by using distilled water the same methods are followed to prepare the base solution of ascorbic acid. The sample is prepared by using the electro thermal method (thermostat) with temperature at 80^0C .The copper borate solution is kept in a thermostat were the base solution of ascorbic acid added to the copper solution in a drop wise manner till the white precipitate forms. The precipitate is filtered washed and dried in oven at 100^0C. The precipitate is stored and labeled.

PREPARATION OF IRON DOPED MATERIALS

The pure copper oxide nanoparticles are doped with ferric chloride anhydrate less than100^0C.1-10phenanthraline anhydrate act as a ligand binder which is add to the copperoxide sample solution.0.1 M

of ferric chloride anhydrate where added drop wise to the sample solution which is kept on thermostat. The color of the solution changed, and precipitate settle down. The precipitate filtered, dried. The doped sample is stored and labeled.

TABLE 1: SAMPLE PH, COLOR, VISCOSITY

Sample	pH			Precipitate (color)	Viscosity
	mL	Initial	Final		
Copper oxide nanoparticles	50	6	8	Nil	Liquid
	100	8	9	White	
	150	9	11	White	
Copper oxide doped with Fe	50	6	8.5	Black	Liquid
	100	8.5	9.3	Brown	
	150	9.3	11	Brown	

RESULT

X-RAY DIFFARACTION (XRD)

XRD is used as a fingerprint region for inorganic material used (crystal impact match 2 and diamond 3) software to draw structure. The blue line shows the observed data the red line shows matched data the colors represent for each match in the doped sample.

Effect of Doping

In our study we used CuO_2 were to study the magnetic nature of the sample by using group theory based computational method. The lattice arrangement of CuO_2 shows the cubic strictures of the particles and the Pnma space group and the atomic distance at 1.9711Å for Cu-O band, 1.8808 Å for Fe-O band 1.9711Å for Fe-Cu band. The XRD shows the high intensity and d-value at 5.047Å this shows the sample is high purity (96-152-5968 ref data number). The atomic distance shows the practice is arranged in the perfect grain size and shape. The hkl value of the high- intensity peak with d-value as 5.047 (101) and second high-intensity peak with have d-value as Å, and hkl value as (200) the two hkl value shows the samples are in 99% purity and perfect arranged size according to the grain size the sample are formed less than 100nm that shows the in SEM report. The size of the unit cell is complete match with reference data.

Magnetic nature is studied through books Magnetic Group Table 1, 2 and 3-Dimensional Magnetic Sub periodic Groups and Magnetic Space Groups Daniel B. Litvin., book from the symmetric calculation spins aligned within the is found to be little ferromagnetic. in the octahedral environment induces a lower crystal symmetry and breaks the inversion symmetry to form a polar structure, exhibits antiferromagnetic behavior with TN of ~22K. When Further compositional modification studies of CuMO (M = Cr, Fe, Mn) series are in progress to validate symmetry breaking principles to discover new multiferroic materials

TABLE-2: CELL PARAMETER FOR SAMPLE CELL

Cell Parameter	Angstrom[Å]
A	7.51520Å
B	6.39480Å
C	7.17160Å

TABLE -3: D-VALUE & HKL VALUE

2 theta	d[Å]	hkl value	Ref, hkl for CuO_2
17.55	5.047	101	110
18.29	4.848	011	112
21.81	4.091	111	111
23.54	3.776	200	002
26.65	3.342	201	020
27.667	3.2217	102	113
37.913	2.3712	301	022
47.45	1.9147	213	112

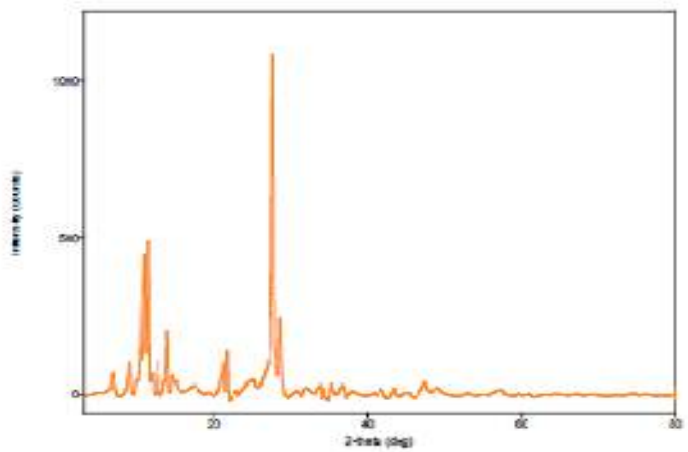

Fig1. Smoothed background data for XRD

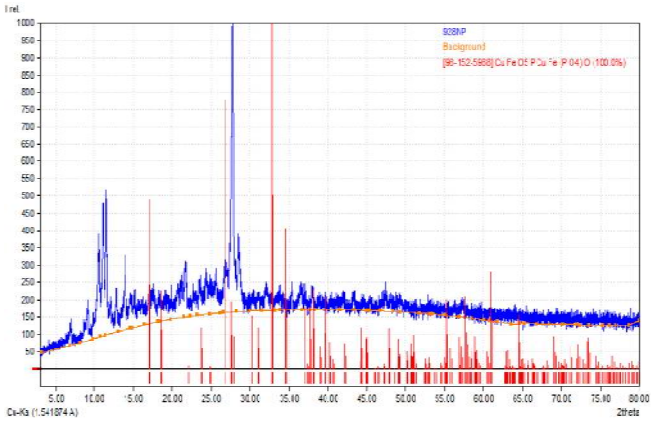

Fig2. Interpret XRD data

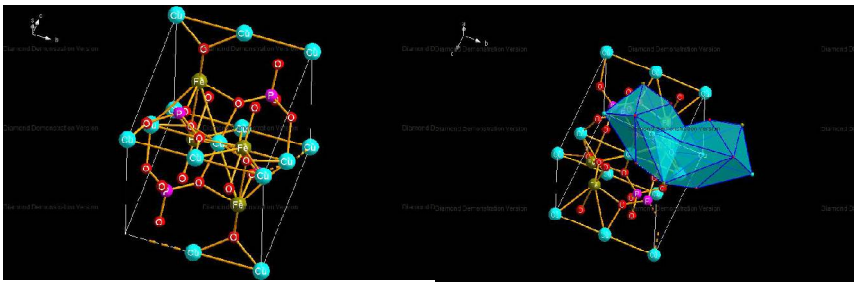

Fig3. Structure and magnetic symmetry activity of CuO2 by diamond software

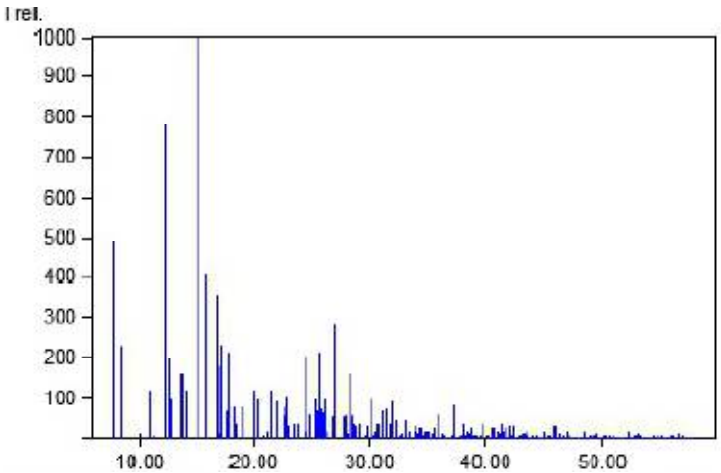

Fig 4. Reference peak of doped material

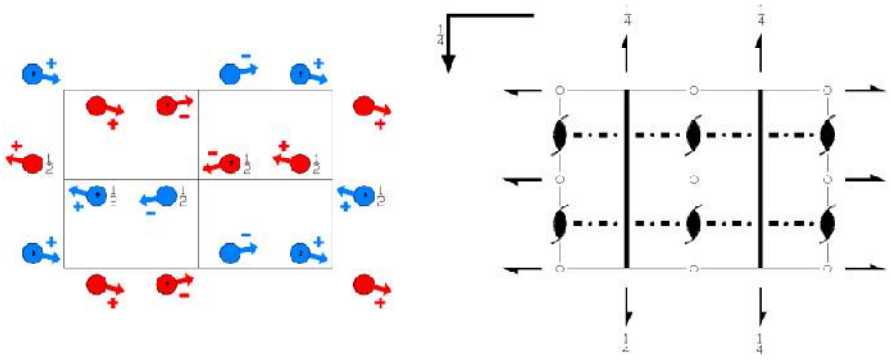

Fig5. Magnetic group table for Pnma space group

SCANNING ELECTRON MICROSCOPY (SEM)

It's used to find the shape and size of the particle. The SEM image of the sample shows of Fig (6 a,b,c) from the image it concluded out the morphology pure particles in a spherical shape, dopped nanoparticles are formed spherical shape and size of the particle. The particles are formed in a spherical shape. The particle is not equally distributed. The size varies from 20-60nm. It may be due to environmental factors like far atmospheric moisture etc. From the image the average particle size is 20-60nm.

Effect of surfactant in size formation

We can often change the characteristics of suspension by understanding how individual colloids interact with one another. We may want to maximize the repulsive force between them to keep each particle discrete are prevent them from gathering into large, faster agglomerates. The attached counter ions in the solution storm layer and the charged atmosphere in the diffuse layer is referred to as the double layer. The thickness of the layer depends upon the type and concentrations of ions in solution (zeta meter .inx). The double-layer formed to neutralize the charged colloid. When we use PEG as a surfactant it increases the viscosity of the solution the increasing viscosity decrease the interatomic colloidal particles. And increase the double layer thickness to this few presents of PEG to the solution medium reduce the surface tension of the solution medium and decrease the particle size.

Effect of doping

When the doping takes place, the impurity added to the parent material due to the impurity, the lattice arrangement of the parent material changed. When adding a known impurity to the parent material, the lattice disorder, takes place. It's due to lattice disorder. The morphology of the parent material was changed. In the present study, Cu and Ni used as a doping material and CdO were used as the parent material. The atomic radius of Cu is higher than Cd, so the doping takes place in a good manner. The lower atomic radius gives the best result in doping and from lattice disorder this lattice disorder gives the change in morphology.

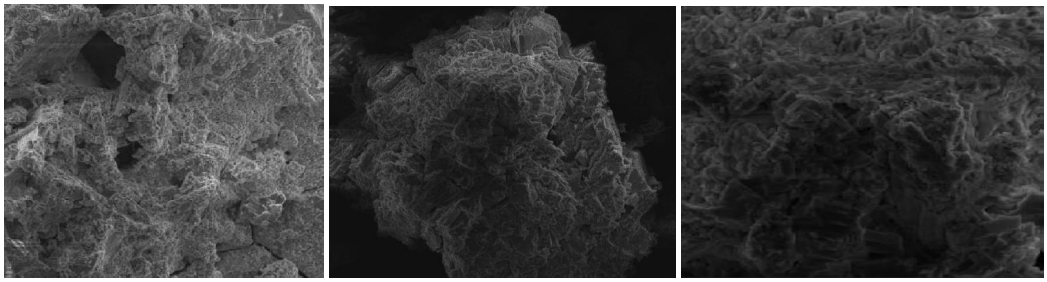

Fig -6 SEM images

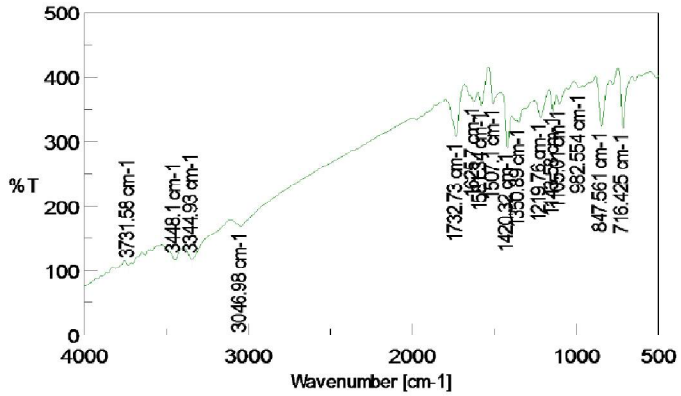

Fig 7 - FTIR Spectrum for Sample

FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

FTIR is used to identify the functional group of the prepared Nanoparticle. The sample shows absorption at 716cm-1 847cm-1,982cm-1,3344cm-1,716cm-1 normally adsorption shows in 2800 -3600cm-1 is due to the removal of OH molecule.716cm-1may correspond to the Cu-O bond vibrational frequencies,847cm-1the additional Cu–O–H bonds, 982cm-1can be attributed to the C–O–C/secondary C–OH bonds,3344cm-1O–H/N–H stretching groups of macromolecular association,716cm-1indicates the presence of Fe_2O_3.

CONCLUSION

Copperoxide nanoparticle was prepared by using electro thermal method. The CuO_2Nanoparticle are characterized by using X-ray diffraction (XRD), scanning electron microscope (SEM), and Fourier transform infrared spectroscopy (FTIR). The XRD confirmed the atomic distance, d-value and hkl value of the sample for the Fe doped copper oxide nanoparticle. From XRD results, magnetic nature studied through symmetric calculation spins aligned within the (a,c) plane of the monoclinic unit cell, forming an angle Θ of 55(2)◦with respect to the a axis. Releasing the constraints did not lead to any noticeable improvement in magnetic moment; all magnetic structures can be viewed as pseudocubic arrangements of magnetic Cu+cations with a G-type antiferromagnetic structure. The SEM image confirmed the spherical shape for Fe doped CuO_2 Nanoparticle was confirmed. The sample is formed less than 100 nm which shows in the report. The lower atomic radius gives the best result in doping and form lattice disorder, the lattice disorder gives the change in morphology. The FTIR confirmed the Cu-O stretching mode demonstrating the existence of Cu-O bond among CuO_2 structure is 541 cm^{-1}, the elimination of OH in Cu(OH) into CuO doping with Fe confirmed by the doping 719 cm-1 is assigned for Fe-O stretching mode of FeO lattice, 1092 cm^{-1} is assigned for O-H bonding vibration joined with Mn atoms. 1409cm^{-1} was assigned for C-H-O bonding mode asymmetrical and symmetrical stretching peaks confirm the presence of PEG in the sample which is used as a capping agent or surfactant, the doped material for the following peaks are assigned and confirmed the doping.FTIR is used to identify the functional group of the prepared Nanoparticle. 716cm^{-1}may correspond to the Cu-O bond vibrational frequencies, 847$cm^{-1}$the additional Cu–O–H bonds, 982cm^{-1}can be attributed to the C–O–C/secondary C–OH bonds,3344cm^{-1}O–H/N–H stretching groups of macromolecular association,716cm^{-1}indicates the presence of Fe_2O_3.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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