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Exploring Characteristics of CuO Nanoparticles by Sol-Gel Method

Avneesh Kumar[1], Lavli Rana[2]
[1]Department of Physics, SV Govt. College Ghumarwin, (H.P), INDIA
[2]Department of Physics, NSCBM Govt. College Hamirpur, (H.P), INDIA

***Abstract*—In this article, production of Copper oxide nanopaticles and its lattice parameters are reported using sol-gel method. The structural & crystallite size studies were performed by utilizing X-ray diffraction. The identification of monoclinic structure of CuO nanocrystallite is ascertained. X-ray diffraction (XRD) results indicates that the c rystallite size is in 20-34nm range with average size of 27nm, lattice parameters are a = 3.735 A^0, b = 3.415 A^0, c = 5.9104 A^0 for monoclinic structure of CuO. Here CuO nanoparticles were annealed at temperature 700˚C.**

***Index Terms*—nanoparticles, Precursor, Copper oxide, Sol-gel, X R D**

I. INTODUCTION

CuO nanoparticle is a brownish black colored powder with a density of 6.3-6.4 g/cm^3 and a melting point of 1326˚c. The particle size of CuO is calculated between 1 and 100nm. CuO is a p-type semiconductor with a narrow band gap of 1.4ev and has a monoclinic unit cell. CuO is an anti-ferromagnetic material. It is also exhibiting non-toxicity and excellent chemical stability. In addition, the high availability and low material cost make CuO a potential candidate for diverse applications including gas sensors, solar cell, lithium-ion batteries and field effect transistors Reports suggest that CuO can also be used as an efficient heterogeneous catalyst for reactions including C-N cross coupling of amines with halogenated benzene oxidation of alcohol and benzene to phenol oxidation and nitroarene reduction. There are reports on the fabrication of various nanoscale CuO possessing varying shapes and dimensions such as nanowires, nanosheets using various techniques. The properties of CuO vary strongly on going from bulk to the nanoscale and the properties influences strongly on size, morphology as well as the aspect ratio of the CuO nanostructure. CuO nanoparticles possess various significant properties and have diverse applications. CuO nanoparticles have been used as batteries, catalyst, and gas Sensors, high temperature superconductors and tools for solar energy conversion among others. Also, CuO has a well documented antimicrobial effect with efficiency against bacteria, yeast and fungi. Because of its biocidal and anti-viral properties, these nanoparticles are used as antimicrobial coatings in textile, wound dressings and plastics. Furthermore, CuO nanoparticles have shown anti cancer properties. However, many tests suggest that CuO nanoparticles are more toxic compared to other available metal-oxide nanoparticles. [1-10]

II. EXPERIMENTAL WORK

To synthesise CuO nanoparticles, 0.2M of copper acetate monohydrate and 0.2M of NaOH are weighed using a weighing balance. Then 50mL of distilled water is measured using a measuring cylinder for each sample. Both the copper acetate and NaOH are dissolved separately in 50ml of distilled water with constant stirring for about 30 minutes to ensure complete dissolution. The NaOH solution is then added to the copper acetate solution with constant stirring using a magnetic stirrer for about one hour. After that, a burette is filled with 100ml of polyvinyl alcohol (PVA) and titrated dropwise into the solution containing the copper acetate and NaOH, continuing the constant stirring. This process leads to the formation of gel from sol Fig.1. Then gel dried, and calcinated at about 700 degrees Celsius for 24 hours in a muffle furnace to produce copper oxide nanoparticle. [11-16]

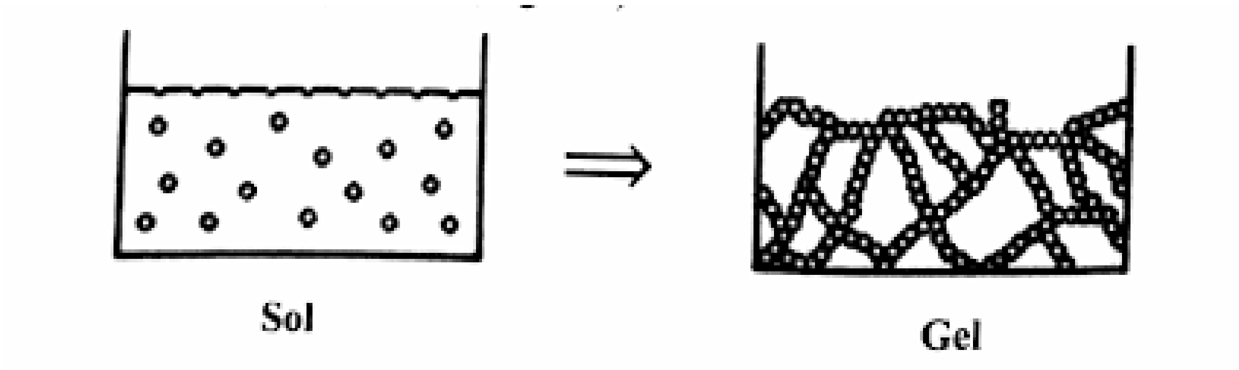

Fig.1

III. RESULT AND DISCUSSION

A. XRD-STUDY:

X-Ray diffraction measurements were carried out to study the crystal structure and crystalline quality. Fig2 represent the XRD pattern of synthesized CuO nanoparticles calcined at 700˚c respectively. All the diffraction peaks could be indexed to crystalline monoclinic structure. The major peaks located at 2θ values correspond to the characteristic diffraction of monoclinic phase of CuO. The CuO nanoparticles were performed using CuKa radiation source of a wavelength λ= 1.54Å and the diffraction pattern studied by changing diffraction angle in the range of 30˚to 80˚. The XRD pattern of CuO nanoparticle synthesised by sol-gel technique annealed at 700^0 C shows intensity up to 20000. The XRD patterns of the products confirm that the formed material is CuO. It can be seen from the XRD pattern that the diffraction peaks are low and broad due to small size effect. All the XRD pattern clearly show the diffraction peaks of the (110),(-111),(111),(-200),(020),(202),(-113),(220) planes.

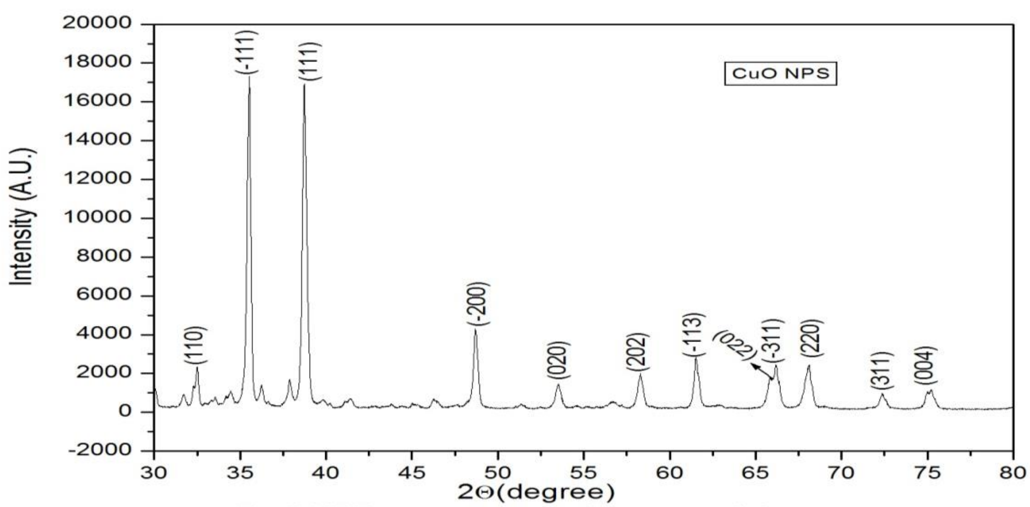

Fig.2 XRD pattern for CuO nanoparticles

The calculated D-values in Table1, confirms that the nanoparticles of CuO have monoclinic structure. It can be observed that by increasing the annealing, intensity rises up to 20000, the peaks became appreciably sharpened which indicates the growth in crystalline size of CuO nanoparticles.The crystalline sizes(D) of CuO nanoparticles were calculated by Debye-scherer equation using full width at half maximum:

$$D=K\lambda/\beta\cos\theta$$

Where D is the crystalline size, β is the broadening of the diffraction line measured at its maximum intensity (FWHM), K is the scherer constant of the order of 0.9 related to crystalline shape and λ is the wavelength of the X-ray beam.

Table1: Crystalline size (D) of CuO NPs:

Angle (2θ)	Θ	θ (Radian)	Cos(θ)	β	β (Radian)	Kλ	βCos(θ)	D	D (nm)	hkl
32.48	16.24	0.283441	0.96	0.241	0.004199	1.3706	0.00403	340	34	[110]
35.50947	17.75	0.309879	0.952	0.252	0.004391	1.3706	0.00418	327.7	32.77	[-111]
38.74405	19.37	0.338106	0.943	0.296	0.005158	1.3706	0.00487	281.7	28.17	[111]
48.70812	24.35	0.425059	0.911	0.289	0.005043	1.3706	0.00459	298.3	29.83	[-200]
53.51382	26.76	0.466996	0.893	0.348	0.00608	1.3706	0.00543	252.5	25.25	[020]
58.29035	29.15	0.508679	0.873	0.353	0.006168	1.3706	0.00539	254.3	25.43	[202]
61.54886	30.77	0.537115	0.859	0.338	0.005903	1.3706	0.00507	270.3	27.03	[-113]
68.06035	34.03	0.593939	0.829	0.457	0.007972	1.3706	0.00661	207.4	20.74	[220]
							AVG=D		27.90nm	

IV. LATTICE STRUCTURE:

Copper oxide is an important transition metal oxide with **monoclinic structure.**

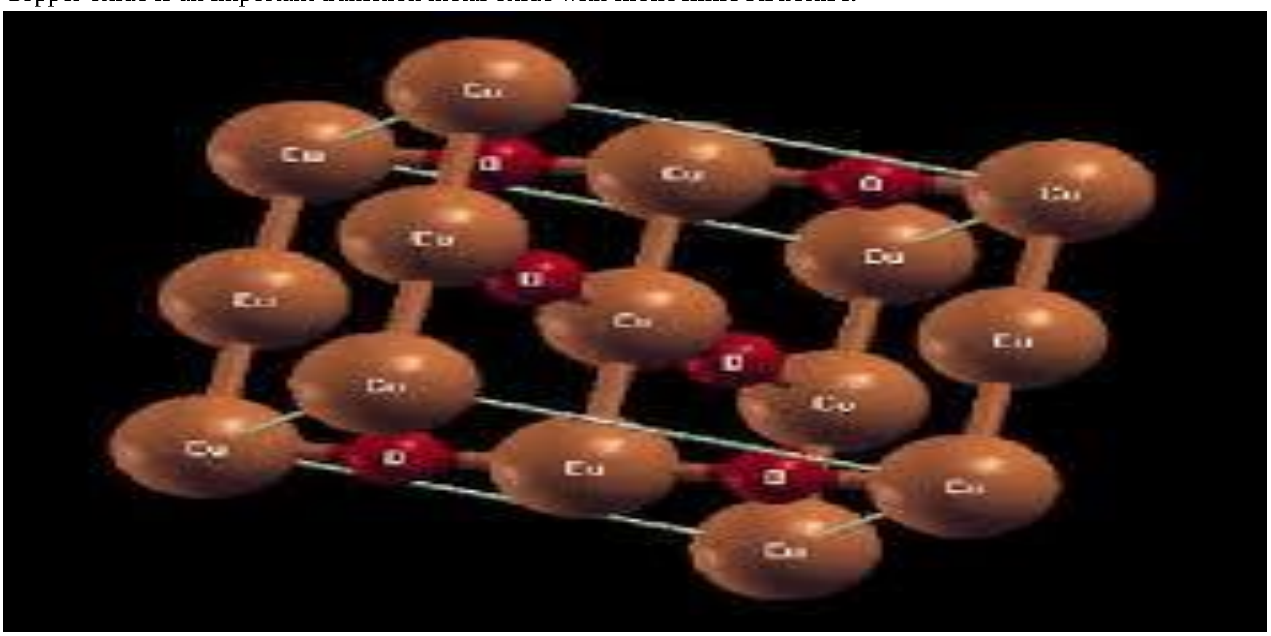

Fig.3

Formula used: $\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$. (1)

For monoclinic structure a≠b≠c

For plane (-200); here h=-2, k=0, l=0

So, $\frac{1}{d^2} = \frac{(-2)^2+(0)^2+(0)^2}{a^2}$

$\frac{1}{d^2} = \frac{4}{a^2}$

$4d^2 = a^2$ …………………………(2)

According to Bragg's law concept – Bragg's law relate the angle θ to the wavelength of x-rays and the interlayer distance'd' between the planes of atoms/ions/molecules in the crystal lattice.

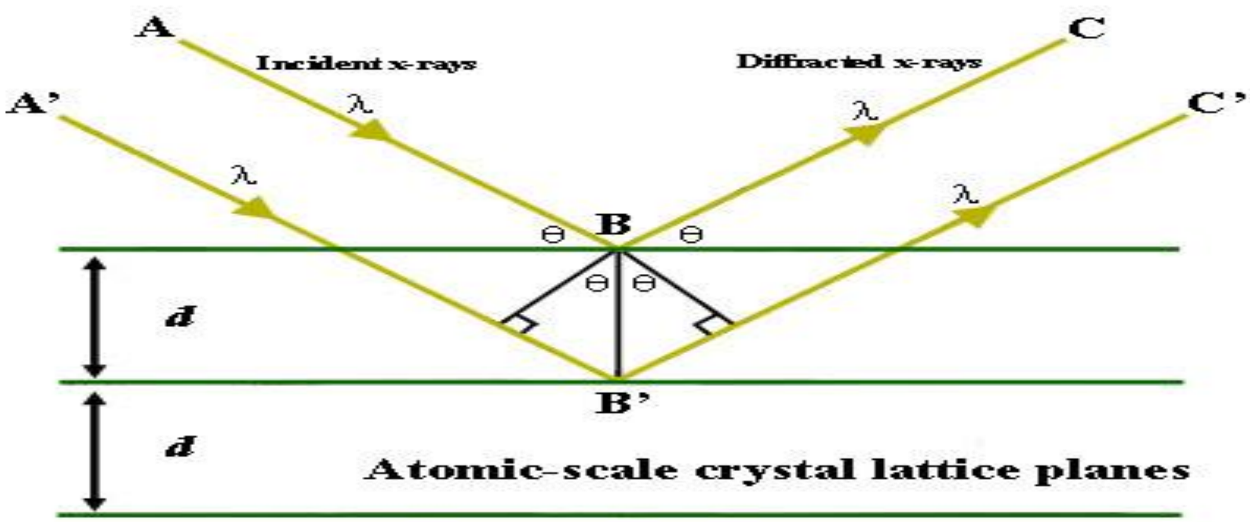

Fig.4

$n\lambda = 2d\sin\theta$

Or $d = \frac{n\lambda}{2\sin\theta}$ ……………... (3)

Here n=1, λ=1.54

$d = \frac{1\times1.54}{2\sin24.35}$

Or $d = \frac{1.54}{2\times0.412}$

Or $d = \frac{1.54}{0.824}$ = 1.868

Or $d^2 = 3.489$………………… (4)

Put (4) in (2)

$4\times3.489 = a^2$

Or $a^2 = \sqrt{13.956}$

Or **a = 3.735** ………….. (A)

Now for plane (020)

Eqn (1);

$\frac{1}{d^2} = \frac{(2)^2}{b^2}$

Or $\frac{1}{d^2} = \frac{4}{b^2}$

Or $4d^2 = b^2$ ……………….(5)

Bragg's law:

$n\lambda = 2d\sin\theta$

Or $d = \frac{n\lambda}{2\sin\theta}$

n=1, λ=1.54

So, $d = \frac{1\times1.54}{2\sin26.76}$

Or $d = \frac{1.54}{2\times0.4508}$

$d = \frac{1.54}{0.9016}$ = 1.7080

Or $d^2 = 2.917$ ………….. (6)

Put eqn.(6) in (5) ;

$4\times2.917 = b^2$

Or $b^2 = 11.669$

Or $b = \sqrt{11.669}$

Or **b = 3.415** …………..(B)

Now for plane (202)

$\frac{1}{d^2} = \frac{4}{a^2} + 0 + \frac{4}{c^2}$

Or $\frac{1}{d^2} = \frac{4}{a^2} + \frac{4}{c^2}$

Or $\frac{1}{d^2} = \frac{4}{13.950} + \frac{4}{c^2}$

Or $\frac{1}{d^2} = 0.286 + \frac{4}{c^2}$…… (7)

From Bragg's law:

$d = \frac{n\lambda}{2\sin\theta}$

n=1, λ=1.54

So, $d = \frac{1\times1.54}{2sin29.15}$

Or $d = \frac{1.54}{2\times0.4873} = \frac{1.54}{0.9746} = 1.5801$

Or $d^{2=} = 2.4967$ ....(8)

Put this value in eqn. (7)

$$\frac{1}{2.4967} - 0.286 = \frac{4}{c^2}$$

Or $0.4005 - 0.286 = \frac{4}{c^2}$

Or $0.1145\ c^2 = 4$

Or $c^2 = \frac{4}{0.1145} = 34.934$

Or $c = \sqrt{34.934}$

Or **c = 5.9104** .... (C)

Hence lattice parameters are a = 3.735A^0, b = 3.415 A^0, c = 5.9104 A^0

IV. CONCLUSIONS

Nanocrystalline CuO nanoparticles were synthesised by inexpensive sol gel method. The identification of monoclinic structure of CuO nanocrystallite is confirmed. X-ray diffraction (XRD) results indicates that the c rystallite size is in 20-34nm range with average size of 27nm, lattice parameters are a = 3.735 A^0, b = 3.415 A^0, c = 5.9104 A^0 for monoclinic structure of CuO. Here CuO nanoparticles were annealed at temperature 700˚C.

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