MANTECH Publications

Journal of Research in Physics and Applied Sciences
Volume 5, Issue 1, January-June 2022

Effect of Copper Doping on Structural, Optical and Electrical Properties of Barium Titanate Nano particles

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Abstract

This paper reports the structural and electrical properties of copper doped Barium titanate ($BaTiO_3$). Different concentrations of copper have been introduced into $BaTiO_3$ to get a stoichiometry $BaTi_{(1-x)}Cu_xO_3$. The X-ray diffraction, Fourier transformed infrared (FTIR) spectrum of the samples doped with different compositions of CuO are recorded and analyzed. The purpose of this work is to throw some light on the influence of Copper on the structural and electrical properties of $BaTiO_3$

Keywords: *Barium Titanate, Nano particles, Fourier Transformed Infrared, samples doped*

INTRODUCTION

The development of lead free hybrid materials with tailored properties is very much essential to address the present issues of the energy crisis. The spontaneously polarized materials (ferroelectrics) are the perovskites of the type ABO_3. The key characteristics of these perovs kite materials often have low carrier recombination probability and high carrier mobility, the diffusion distance, low band gap energy and lifetime of carriers are long, which leads to the excellent performance in various optoelectronic applications [1-3]. Barium titanate ($BaTiO_3$) is one of the best known Perovskite ferroelectric compounds due to its like low dielectric losses, high values of the dielectric permittivity and high electromechanical coupling coefficients.

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The three different crystalline forms of barium titanate are cubic, tetragonal and hexagonal, in which the most useful one is the tetragonal polymorph because of its excellent ferroelectric, piezoelectric and thermoelectric properties. The polarization and crystal structure of $BaTiO_3$ were strongly affected by the temperature. The Curie's temperature (T_c) for all Cu doped $BaTiO_3$ was found to be in the range of 120°C to 125°C. Below the Curie temperature, the crystalline cell is suffering a series of changes: to tetragonal (at 1200C), from tetragonal to orthorhombic (at 00C) and from orthorhombic to rhombohedra (at –900C) in which the material has ferroelectric properties [4].

Ferroelectrics are materials which have the outstanding property of possessing spontaneous electric polarization, the reversibility of the permanent polarization by an electric field.

Due to their possessing large piezoelectric values, make them more attractive in different piezoelectric application. $BaTiO_3$ has been a ferroelectric and piezoelectric with an extensive application. Copper oxide is usually added as a sintering aiding BaTi03 based capacitor compositions. Sample of Copper doped Barium Titanate was prepared via Solid State Reaction technique, replacing titanium with copper such that its stoichiometry is $BaTi(1-x)Cu_xO_3$

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EXPERIMENTAL

The starting materials were analytical reagent grade $BaCO_3$, $CaCO_3$, TiO_2 and CuO. 0.25M is to be prepared. The weights of different compounds were found out analytically, corresponding to different concentrations of CuO (0.02M, 0.04M, 0.06M & 0.08M) .The mixtures were weighed using an electronic balance of accuracy 0.0001. Weighed mixtures of the four components were homogenized by grinding. The grinding was done on a clean agate mortar for 4 hours.

The grounded mixture was then passed onto a sieve of 75 micron hole size and the mixture was sieved mechanically. Particles of size less than 75 micrometers managed to pass through. The sieved mixture was then heated at 700C for 4 hours in a preheated furnace followed by a furnace cooling. X ray diffraction (XRD) and FTIR spectrum of the mixture was then studied. The film was developed on a glass plate and on ITO (Indium Titanium Oxide) glass plate. The plate is then subjected to heating at 800C. The conductivity and resistivity of the mixture were studied.

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RESULTS AND DISCUSSIONS

X-Ray Diffraction Studies

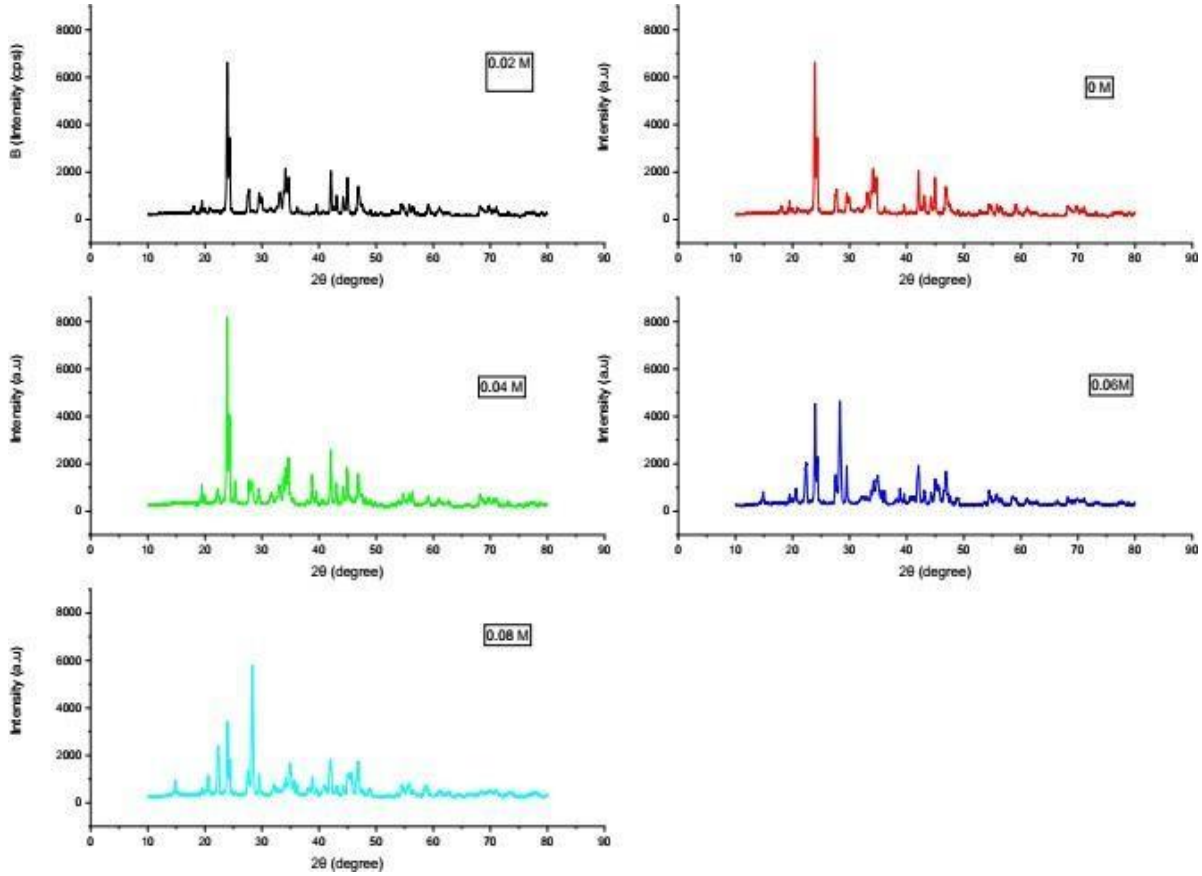


Figure 1. X-Ray Diffractograms Of Ba1-Xcuxtio3; X= 0,0.02,0.04,0.06 And 0.08

X-ray diffraction (XRD) is a versatile and non-destructive technique that yields the detailed information about the chemical composition and crystallographic structure of different materials. X-ray diffraction pattern of samples having different concentrations of copper is analyzed. Peaks were obtained in the X-ray spectrum and the highest peak was obtained in the 2-theta range from 22-24^0 of angle. The crystalline size lies between 20 and 30 nanometers in the samples.

Table: X-Ray Diffraction Values of Various Concentration of Cu.

Cu-0M			
2 theta	**FWHM**	**Crystalline size D (nm)**	**average D (nm)**
23.93079	0.24561	33.06350765	27.84351875
24.33349	0.24244	33.52099802	
42.08678	0.25073	33.94871882	

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34.16933	1.27206	6.533529321	
44.97627	0.26743	32.15083996	

Cu- .02M			
2 theta	**FWHM**	**Crystalline size D (nm)**	**average D (nm)**
23.88765	0.2145	37.85585475	30.67481465
24.29705	0.21314	38.12646161	
42.04417	0.22898	37.1680728	
34.11463	1.40763	5.903414327	
44.93714	0.25049	34.32026977	

Cu-.04M			
2 theta	**FWHM**	**Crystalline size D (nm)**	**average D (nm)**
23.90972	0.21322	38.0846629	28.71428213
24.30321	0.22355	36.3514564	
34.26876	1.36896	6.072683962	
42.05016	0.25528	33.33953421	
44.95372	0.28925	29.7230732	

Cu-.06M			
2 theta	**FWHM**	**Crystalline size D (nm)**	**average D (nm)**
22.35678	0.36942	21.92063224	25.40884079
23.97461	0.27768	29.24728777	
28.31923	0.35442	23.11724835	
42.02956	0.40902	20.80663144	
29.51164	0.20042	40.99005386	
46.86139	0.52887	16.37119108	

Cu-.08M			
2 theta	**FWHM**	**Crystalline size D (nm)**	**average D (nm)**
22.3459	0.37034	21.86576677	20.22486715
23.97562	0.27164	29.89766628	
28.3176	0.32109	25.51678893	
34.85451	1.22699	6.786112269	
41.99048	0.41081	20.71325934	
46.82247	0.52246	16.56960933	

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Fourier Transform Infrared Spectroscopy

Fourier transform infrared spectroscopy is a technique that is used to obtain the infrared spectrum of absorption and emission. It is used to find different functional groups in the sample. Absorption bands are grouped into 2 types: group frequencies and fingerprint frequencies. Group frequencies are characteristics of small groups of atoms or functional groups. These bands are seen above 1500cm^{-1} in the infrared spectrum. Fingerprint frequencies are highly characteristic of molecules as a whole. These types of absorbance are usually seen below 1500cm^{-1} in the spectrum. Here the fingerprint region peaks are obtained mainly at 5 positions, 1430±5cm^{-1}, 1270±20cm^{-1}, 1050cm^{-1}, 860±10cm^{-1} and 675cm^{-1} in all the 5 graphs (O-Ti-O stretching modes)[5-6]. The FTIR spectrum of all the samples is coupled together and is plotted with transmittance in Y-axis against wave number (cm^{-1}) in X- axis.

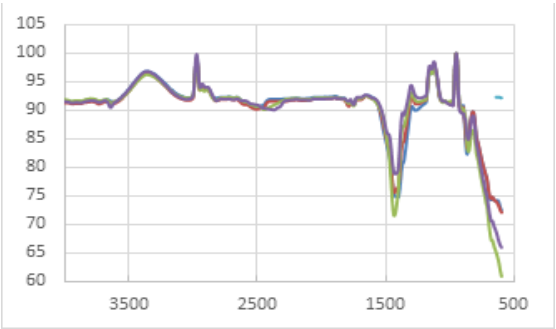


Figure 2: FTIR analysis of Cu doped BaTiO3

Conductivity and Resistivity

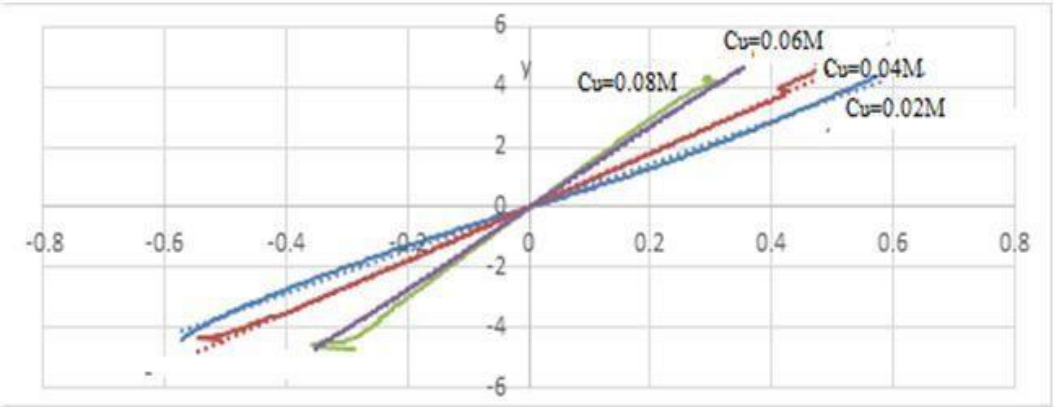


Figure 3 : D.C. Electrical Conductivity

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Determining the D.C. electrical conductivity of a sample is another highly informative macroscopic measurement technique. The graph is plotted with voltage along Y-axis and current along X-axis. The substitution of copper in the place of Barium improves ion transport mechanism could be due to the trapping of holes on Ba-O bonds.

CONCLUSION

In this paper, we have studied the impact of doping on the structural, electrical and spectral properties of the Barium Titanate nanoparticles. Here doping improves the confinement effect. The electrical conductivity studies indication the participation of copper ions and hole conduction by trapping of holes on Ba-O bonds.

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