Structural and Electrical Analysis of Barium Titanium Oxide Nanoparticles

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Abstract :
Nano particles of barium titanium oxide nanoparticle was synthesized and analyzing the structural and electrical parameters of the prepared samples by microwave assisted solvothermal method by microwave oven. Powder X-ray diffraction of the powder was carried out after calcinating the temperature 400°C resulted in. Pure monoclinic structure Ba_2TiO_4 nanoparticles was obtained with lattice parameters, a=6.1458 A°, b =7.6727A°, c=10.5673 A° The particle size was obtained from the studies of X-ray line bordening studies and scanning electron microscopy studies was taken. The electrical parameters were found for Ba_2TiO_4 at 100 Hz to 1 MHz.

Keywords : Ba_2TiO_4, microwave, solvothermal, monoclinic, X-ray diffraction, electrical parameters, scanning electron microscopy.

I. Introduction :

Nanoscience is meant to deal and manipulate the materials particularly, at the molecular level wherein the property modifications may suppose to be emerged. It is obvious that the nanomaterials research is an extension from the level of atoms and molecules to different dimensions of nanostructures [1]. Nanoscience is the branch renders detailed knowledge on the property relationship with particle size and its dimensions. Observations on the borderline of property changes in length scale of particle size are very crucial. This could significantly be useful to understand the property dependence of each material on their molecular level of organisations. The application potential of nanomaterials is significantly rich in wide variety of fields like biomedical, engineering, agriculture, automobiles, military and defence, buildings and infrastructure, etc [1, 2]. The present work is interested to address and discuss the size dependent physical properties of nanosize particles with the help of variety of characteristic tools. The properties interested to explore are belongs to structural, optical, morphological, crystalline and etc. It is one of the novel disciplines developed to approach the materials science. More specifically, to deal the materials whose particle size within the scale of limit, from one to one hundred nanometers (1-100 x 10^{-9}m). Interestingly, this point of length is said to be the "magical point" at which the aspects of human made devices possibly meeting the molecular features belong to the natural world [3]. The preparation of nanomaterials can be accomplished through "bottom-up" or "top-down" methods. Barium titanium oxide is the inorganic compound with the chemical formula Ba_2TiO_4. It is a colourless solid that is of interest because of its relationship to barium titanate, a useful electro ceramic [4]. It is also known as Barium orthotitanate. Barium titanium oxide (Ba_2TiO_4) is barium rich and stable. This material has a high melting point of 1860°C and is unusual as it has Ti^{4+} ions tetrahedrally coordinated to oxygen. It has recentlygained a renewed interest due to its CO_2 absorption properties. Ba_2TiO_4 can effectively remove CO_2 from exhaust gas at high temperature [5].

2. Materials and Methods :

In this present work pure Ba_2TiO_4 nanoparticles were prepared by a facile Microwave oven solvothermal method using domestic microwave oven (operated with a frequency of 2.45 GHz and power 800W). Pure barium titanium oxide nanoparticles were prepared using barium acetate, titanium tetra chloride and urea were taken in 1:3 molecular ratio were mixed and dissolved in 200ml of distilled water then it was stirred well with magnetic stirrer. The dissolved solution was kept in a domestic microwave oven. The colloidal precipitate obtained was cooled to room temperature naturally and washed several times with double distilled water and then with acetone to remove the organic impurities present if only. Then the washed final products were collected and then dried in atmospheric air. The as prepared samples were annealed at 400°C for 1 hour and finally, the products were collected as the yield and the yield percentage was calculated using the relation. The prepared sample was in white colour precipitate. PXRD, SEM image and the dielectric studies via real and imaginary part of complex dielectric permittivity and AC conductivity measurements were carried out within the temperature range of 40 – 150 ºC.

$$\text{Yield percentage (\%)} = \frac{product\ mass}{sum\ of\ masses\ of\ reactant} \text{x } 100$$

3. RESULT AND DISCUSSION

3.1 PXRD Analysis

PXRD analysis is used to determine the crystalline size and lattice parameters of the prepared Ba_2TiO_4 sample. Fig 1 shows the PXRD pattern of the pure Ba_2TiO_4 nanoparticles after heating treatment. The observed peaks could be assigned to the monoclinic phase which is in good agreement to the crystallographic data of Ba_2TiO_4 (JCPDS: 70-1377) [6]. The broadening peaks of the PXRD pattern clearly indicate that the nano crystalline nature of the samples. The average crystallite size was calculated by Debye-Scherer formula. [7]

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

Where D is the mean crystallite size, K is the size factor (0.9), λ is the wavelength of incident beam, β is the full width half maximum (in radian) and θ is the Bragg reflection angle. The average particle size was found as 6 nm. From the indexed PXRD pattern the peaks obtained in the pattern of Ba_2TiO_4 nanoparticles matches well with the monoclinic phase of Barium titanium oxide with lattice constants a=6.096, b=7.681, c=10.549. (Bland 1961, WU & Brown 1973 and Saalfeld 1972,1975). When compared with JCPDS diffraction peak, our diffraction peak shows the small shift in diffraction angles along with the intensity variation. It is due to the effect of crystalline size. The lattice parameters (a, b, c) of the pure sample is calculated for the monoclinic crystalline structure. The values of the sample was a=6.1458 A^o, b =7.6727A^o, c=10.5673 A^o. According to scherrer's equation, the value of crystalline size was 6 nm.

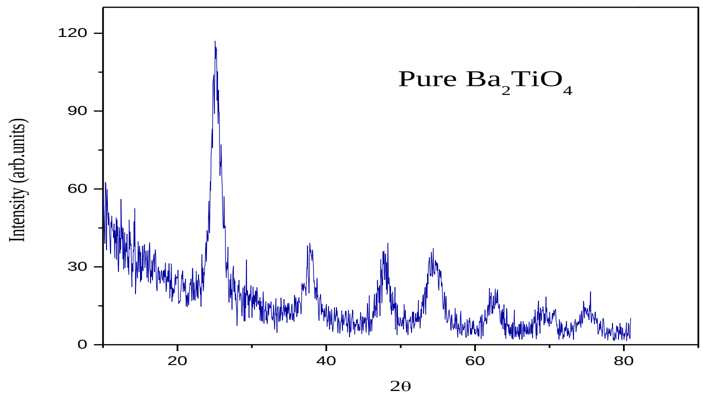

Fig 1 : PXRD pattern of Ba_2TiO_4 nanoparticles

3.2. SEM Analysis :

SEM is the process of the sample to scanning with an electron beam to produce the magnified images. This is useful in qualitatively determining chemical composition and crystalline structure. It exhibits black and white three dimensional images. The SEM micrographs were recorded with scanning electron microscope using Jeol JSM 6390 for all the prepared samples. SEM micrographs are shown in **Fig. 2.** The pure Ba_2TiO_4 sample was agglomerated also have spherical shape and narrow size distribution. It reveals that the morphology is slightly altered. This may due to the particle size of Ba_2TiO_4 sample was low.

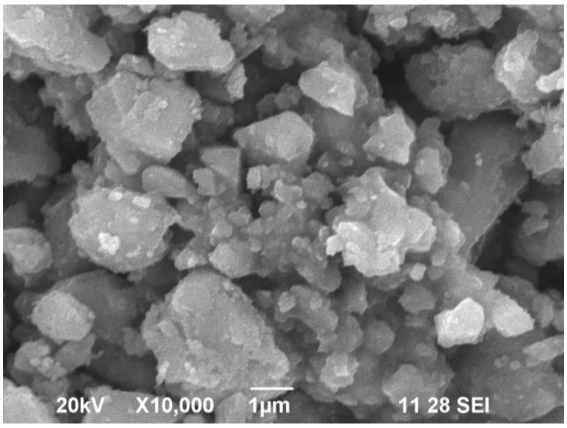

Fig 2: SEM image of pure Ba_2TiO_4

3.3. Electrical analysis :

Dielectric studies :

AC electrical parameters were carried out LCR meter in the temperature range 40 – 150°C at various frequency. 100 Hz to 1MHz were the various frequencies to find the dielectric studies. The parameters such as dielectric constant, dielectric loss and AC electrical conductivity of the pure sample. The dielectric constant was calculated using the relation, ε_r = C/C0. Where, C is the measured value of capacitance in the strong accumulation region, C0 is the capacitance of an empty structure and tan δ is the dielectric loss [8][9]. The variation of dielectric constant with frequency and temperature was shown in Fig 2 - 4. It was observed that the dielectric constant and dielectric loss factor values increase with increase in temperature and decreases with increase in frequency for all the proposed samples [10][11]. The increase in (ε_r) with increase in temperature mainly due to the oriental polarization [12]. The dielectric constant (tanδ) of complex dielectric permittivity decreases with increase in frequency indicates that the (tanδ) values highly dependent on the frequency of the applied field. The high values of (tanδ) at low frequencies is attributed to the charge lattice defect of the space charge polarization [13][14].

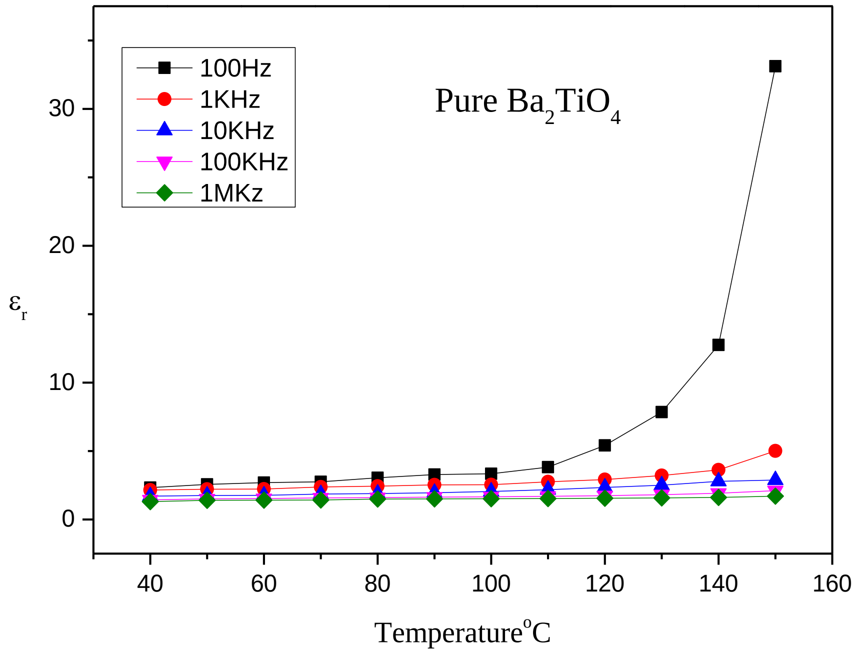

Fig 3: Dielectric constant of pure Ba_2TiO_4 nanoparticles

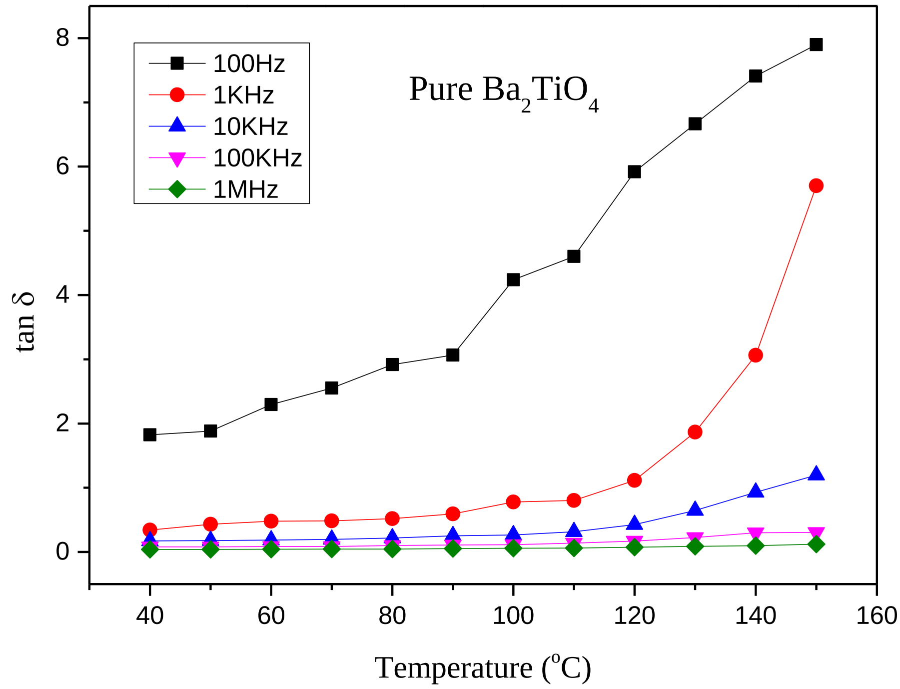

Fig 4: Dielectric loss factor of pure Ba_2TiO_4 nanoparticles

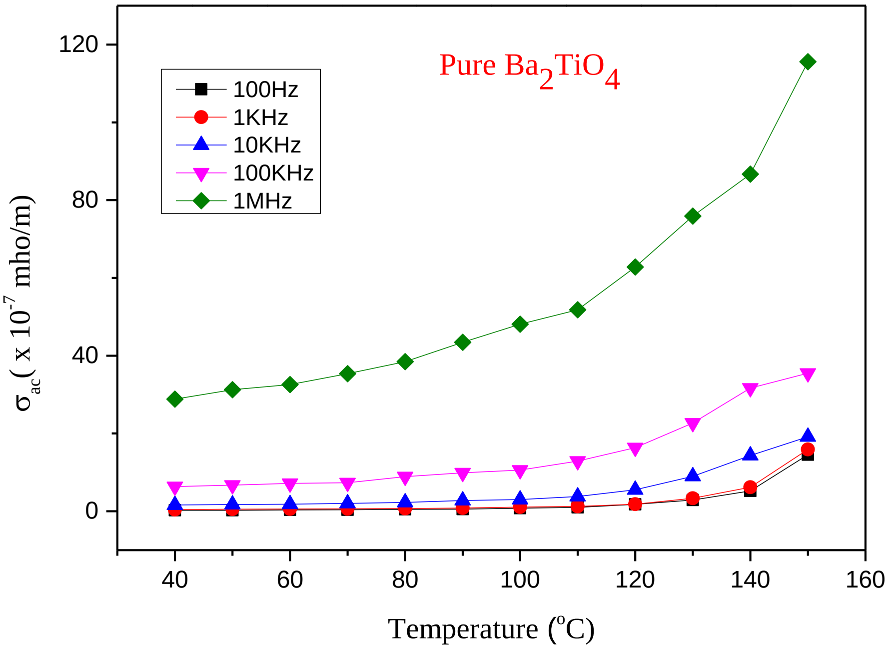

Fig 5: AC Electrical conductivity of pure Ba_2TiO_4 nanoparticles

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