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Syntheses ($Ba_x Fe_{1-x} Ti O_4$) Nano size and Study Crystal properties, Optical Energy Gap and Optical & Electrical Conductivity

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Abstract
In this work, The ($Ba_xFe_{1-x}TiO_4$) (x=1, 0.1, 0.2, 0.3, 0.5, 0.6, 0.7,08, 0.9 and 0) were prepared by the sol- gel method. The influence of Fe concentration on the structural and optical properties of the samples were studied by using x-ray diffraction (XRD), and UV-VIS spectroscopy. The X-ray diffraction (XRD) analyses shows that for all samples the average Nano size decrease with decreasing of iron concentration. UV-visible absorption spectra showed that the observed value of the energy gap decreass from (2.074) eV to (2.046) eV as iron concentration decrease. The conductivity increases when Fe concentration increases shorter wavelengths and decreases at long wavelength.

Key words: *Nano size, dielectric, energy gap, conductivity, crystal size, x-ray diffraction, Ultra violet.*

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I. Introduction:

The discovery of electricity made radial change in human life. Electricity is now widely used to operate electronic devices like mobile phones, computer, beside air conditions and electric lamps. The discovery of electricity enhance electronic applications appreciably. This encourages researchers to search for composite materials that electronic components materials more efficient. The oldest techniques are based on mixing different elements such mixing and doping. Perovskite is considered one of the most promising materials of the twenty-first century. In the past few decades, the perovskite has attracted broad attention and made great progress in energy storage, as well as optoelectronic devices due to its superior photoelectric and catalytic properties [1]. All materials with ABX3 structure are collectively referred to as perovskite materials, where A and B are cations, A is usually an alkaline or rare earth element, and B transition metals. While X is anion may be oxygen, or halogen. These perovskites are classified in three categories: inorganic oxide perovskites, alkaline metal halide perovskites and organic metal halide perovskites with oxide or halide anions [2, 3, and 4]. Materials with perovskite-type are of considerable interest in matter sciences as well as advanced materials research and applications. This is due to their wide array of properties the ample variety of functional properties of the perovskite materials arises from the range of different crystal structures they may adopt by incorporating different alkaline earth, rare-earth, and transition metal ions [5]. Perovskite materials are widely used for scientific and technological applications. It can be applicable to design developed electronic devices due to its remarkable electronic properties. The perovskite materials are well known for several significant properties like ferroelectric, piezoelectric, magneto caloric and optical, dielectric and ferromagnetic properties etc. [1, 6]. Basically, properties of the perovskite material are depended on the structure, composition and other several factor like a synthesis method, synthesis condition and synthesis parameters. A wide range of perovskite material properties can be adjusted by structuring at the Nano scale. Generally, Nano-sized perovskite are prepared by solid-state reactions, a hydrothermal reaction etc. [7]. Sol-gel auto combustion has recently become a very popular technique due to simple process, low sintering temperature, and time and energy consumption than other traditional methods [8]. Therefore, the sol-gel method is employed to improve properties with more

homogeneity and constricted particle distribution this will be making an impact on structural, electrical and optical properties of perovskite. The family of perovskite materials has all kind of compounds including metals, semiconductors, insulators, and superconductors which make them applicable in various technologies. Nano-sized dielectric perovskite have attracted the considerable attention of scientists and technologists due to its multi-functionality. That possess high dielectric constant, and good optical and thermal reliability. Thus, improve their properties which will be useful for the various technologies. It observed that materials which have a high dielectric constant that means possess large energy gap this can cause huge resistivity. So to overcome these issues it is necessary to decrease energy gap, which can be achieved to a certain extent by doping by metal. This follows with exchange in its electric properties such as conductivity [9, 10].

II. Materials and method:

The ($Ba_xFe_{1-x}TiO_4$) (x=1, 0.1, 0.2, 0.3, 0.5, 0.6, 0.7,08, 0.9 and 0) Nano compounds were prepared by the sol- gel method. Barium nitrate [$Ba(NO_3)_{2]}$], Iron(III) nitrate [$Fe(NO_3)_3.9HO_2$] and titanium oxide were used as starting material, distilling water as dissolving medium and nitric acid as adjusting of PH less than 5 PH . First Barium nitrate and iron nitrate were weighted separately, each one followed by the addition of suitable quantity of distilling water to make solution, which was stirred and heated after PH was adjusted to 5.0 at$70c^0$ for one hour. Secondly the two solutions were mixed and added 3.0g of titanium oxide, the product mixture was heated and stirred at $70c^0$ continuously about one hour, the last one was deposited for one day then filtered. Then the solution was slowly evaporated to form sol by continues in heat treatment convert to gel at$150c^0$ after two hours. Finally the gel was dried and grinded to powder. The structural properties were determined by using XRD and Rietveld. Ultra-visible spectrometer (UV) was used to study optical properties.

III. Results and Discussion:

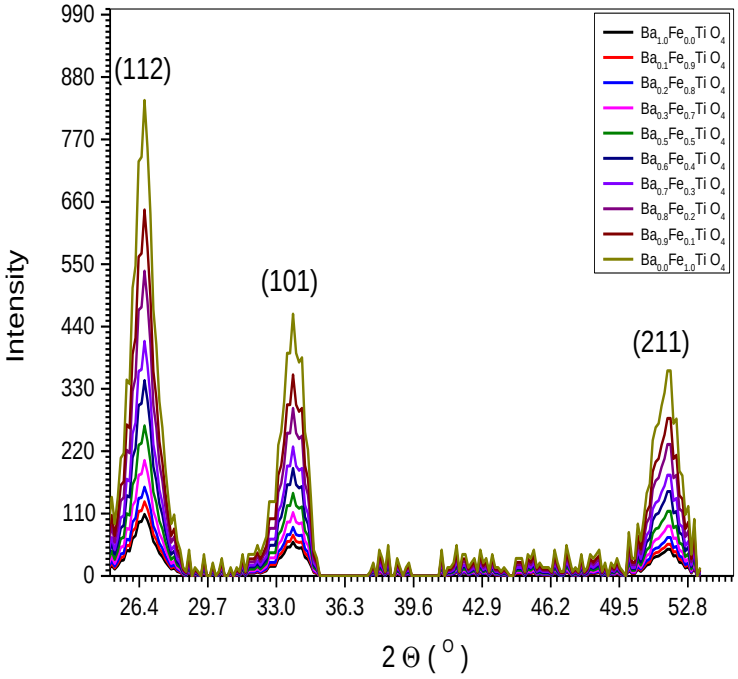

Fig (1) XRD spectrum of all ($Ba_x Fe_{(1-x)} Ti O_4$) samples

Table (1) some crystallite lattice parameter (Average Lattices constant, Xs(nm) d – spacing and energy gap) of ($Ba_x Fe_{(1-x)} Ti O_4$) (x=1, 0.1 ,0.2 ,0.3 ,0.5 ,0.6, 0.7,08 ,0.9 and 0) Molar.

Sample	Average Lattices constant	Xs(nm)	d-spacing	Eg (eV)
$Ba_{0.0}Fe_{1.0}TiO_4$	4.7282	12.6	2.5861	2.074
$Ba_{0.1}Fe_{0.9}TiO_4$	4.7275	12.4	2.5860	2.069
$Ba_{0.2}Fe_{0.8}TiO_4$	4.7273	12.4	2.5859	2.067
$Ba_{0.3}Fe_{0.7}TiO_4$	4.7273	12.3	2.5858	2.064
$Ba_{0.5}Fe_{0.5}TiO_4$	4.7268	11.9	2.5856	2.061
$Ba_{0.6}Fe_{0.4}TiO_4$	4.7263	11.8	2.5455	2.058

$Ba_{0.7}Fe_{0.3}TiO_4$	4.7261	11.7	2.5433	2.055
$Ba_{0.8}Fe_{0.2}TiO_4$	4.7260	10.8	2.5432	2.052
$Ba_{0.9}Fe_{0.1}TiO_4$	4.7256	10.6	2.5431	2.049
$Ba_{10}Fe_{0.0}TiO_4$	4.6104	9.4	2.5430	2.046

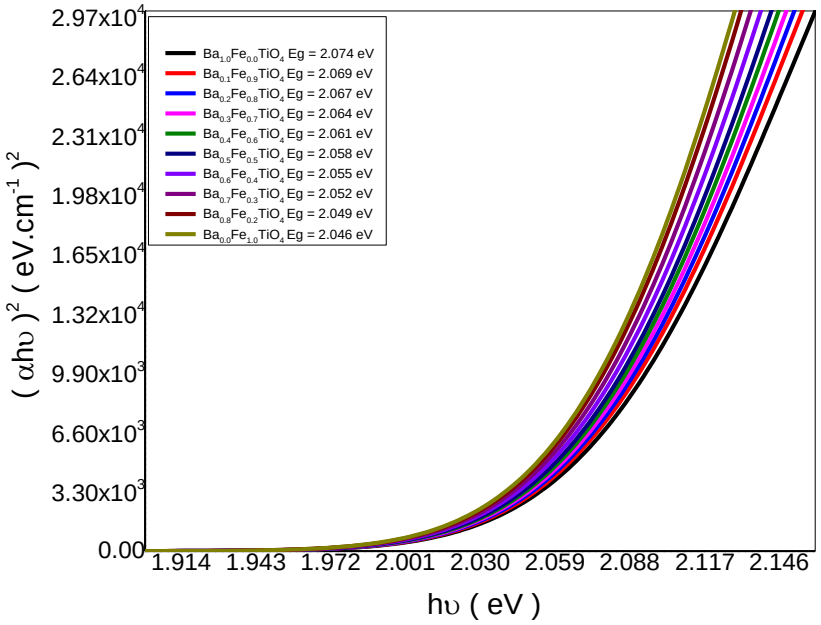

Fig (2) Optical Energy Band Gap spectrum of all (Ba $_x$ Fe $_{(1-x)}$ Ti O_4) samples

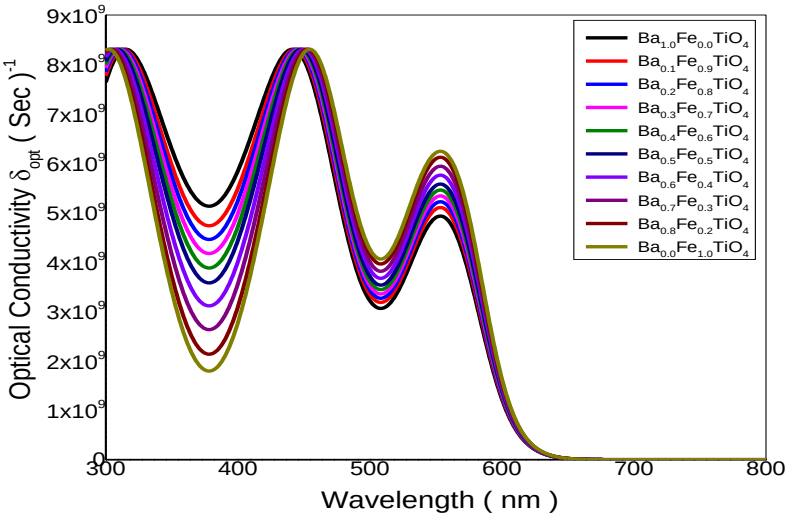

Fig (3) Optical Conductivity spectrum of all (Ba $_x$ Fe $_{(1-x)}$ Ti O_4) samples.

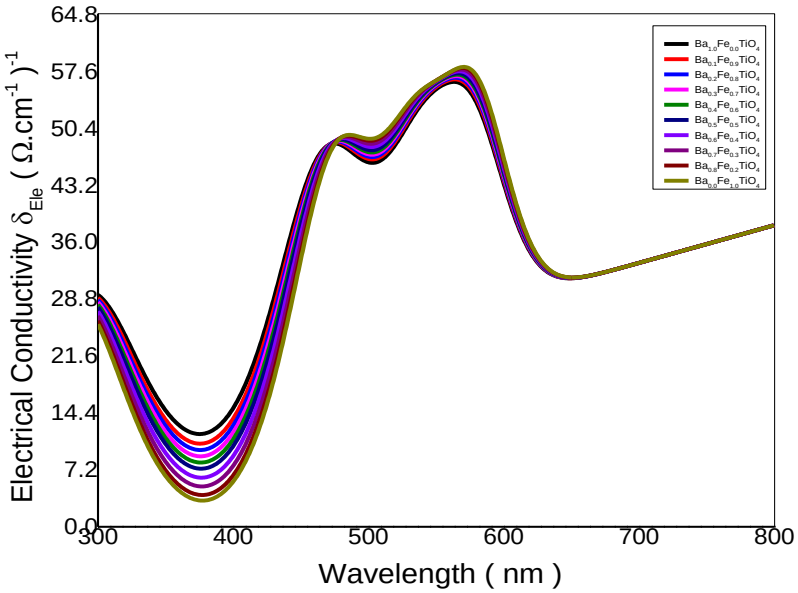

Fig (4) Electrical Conductivity spectrum of all (Ba $_x$ Fe $_{(1-x)}$ Ti O$_4$) samples

IV. Discussion:

The compound ($Ba_xFe_{1-x}TiO_4$) (x1, 0.1, 0.2, 0.3, 0.5, 0.6, 0.7,08, 0.9 and 0) shows some interesting physical properties. Decreasing Fe concentration decrease crystal sizes x and crystal spacing d between adjacent atoms. This may be explained by assuming that decreasing Fe concentration which has atoms acts as magnetic dipoles decreases repulsive magnetic force, which decreases crystal spacing and crystal size as shown in table (1). Figure (2) show the optical energy band gap that calculated by relation $(\alpha h\nu)^n = C(h\nu - E_g)$ where (C) is constant. By plotting $(\alpha h\upsilon)^n$ vs photon energy ($h\upsilon$) as shown in fig.(2) by optical method . Figure (2), indicates that upon decreasing Fe concentration decrease the energy gap. Thus may be related to the effect of Fe on splitting of energy level. This means that decreases the strength of local magnetic field, thus decreases the energy gap. This may be also explained by assuming that the magnetic field generated by Fe acts against the Nano crystal forces that increase and broaden energy bands, thus decreases the energy gap. The optical conductivity is a measure of frequency response of material when irradiated with light which is determined using the following relation, $\delta_{opt} = \frac{\alpha nc}{4\pi}$ where (c) is the light velocity. The electrical conductivity can be estimated using the following relation $\delta_{ele} = \frac{2\lambda\delta_{opt}}{\alpha}$. The high magnitude of optical conductivity ($8.36x10^9$ sec^{-1}) confirms the presence of very high photo- response .The optical and electrical conductivities in figures (3) and (4) shows increase of conductivity upon increasing Fe concentration for shorter wavelengths and the conductivity decreases upon increasing Fe concentration at long wavelength. The former compound are may be attributed to the fact Fe is a good conductor, increasing Fe concentration increase free electrons, thus increases conductivity although the energy gap increases. The latter case may be result from the fact that increasing Fe concentration decreases the energy gap, thus allows more electrons to bridge the energy gap.

V. Conclusion:

The energy band gap decreases as the average Nano size decreases. The conductivity increases upon increasing Fe concentration and the Nano size as well.

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