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The Effect of Fe Concentration on Crystal size, Crystal Spacing, Nano Size, and Absorption Coefficient for ($Ba_x Fe_{1-x} Ti O_4$)

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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. The effect of Fe concentration on the Nano structure and optical properties of the samples were studied by using x-ray diffraction (XRD), and UV-VIS spectroscopy. The X-ray diffraction (XRD) analyses show that for all samples the average Nano size decreases upon decreasing iron concentration. UV-visible absorption spectra shows that decreasing iron concentration increases absorption coefficient. Moreover decreasing Nano size, increases absorption coefficient.

Key words: *Nano size, dielectric, absorption coefficient, crystal size, x-ray diffraction, Ultra violet.*

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I. Introduction:

Nano science is a new branch of physics that deals with isolated particles having nano dimensions (1-1-300 nm). Therefore they can not be described by classical laws. Such small scales can besuitably described by the laws of quantum physics. The behavior and the physical properties of nano systems depends on the nano size, shape as well as the orientation of atoms and molecules. Nanotechnology can thus be used to produce new materials, structures, and systems having new physical properties [1,2]. These materials being significantly modified physical, chemical, and biological properties due to their Nano scale sizes can be used in improving the performance of fabricated devises [3].The nanometer scale is defined as 1 to 100 nm. One nanometer is one billionth of a meter (10 m). The nanomaterial is considered to be a fundamental unit of nanotechnology. Nanomaterials are defined as materials designed to have structural features with at least one dimension of 100 nanometers or less. It can be designed on the surface of a substrate (one dimension), as strands or fibers (two dimensions), or particles (three dimensions) [4, 5]. Nano can be used in electronics, optical communications , cancer therapy, and biofuel production. The application of nanomaterials depends on many factors including their new physical properties, , which provides possibilities for improvement of functionality of nanomaterials [6, 7]. In e electronics one needs components, and integrated systems that have large storage capacity and fast speed.speed.This requires developments in the capacity to measure, organize, and manipulate matter at the Nano scale. The change of geometry and Nano siza and atomic structure and orientation affect physical properties of the nano materials. So there are a wide range of material properties can be modified on the nano scale [8]. several factors like a synthesis method, synthesis condition also affect the properties of the fabricated materials. Various physical and chemical methods of preparation have been developed to achieve nano sizes such as chemical vapors deposition (CVD), sol-gel and physical vapors deposition (PVD) [9, 10]. Moreover modification of Nano materials with metal and nonmetal elements has received much attention and doped nanoparticles exhibit novel properties and according to impurity type [11,12]. Doping with selective elements offers an effective method to enhance and control the structural, electrical and optical properties of Nano materials[13]. The aim of this work is to see how the change of iron concentration affects the physical properties

of the host barium titanium oxide. Secations 2 and 3 are concerned with the materials and discussion, while the conclusion is in section 4.

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 meter . 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:

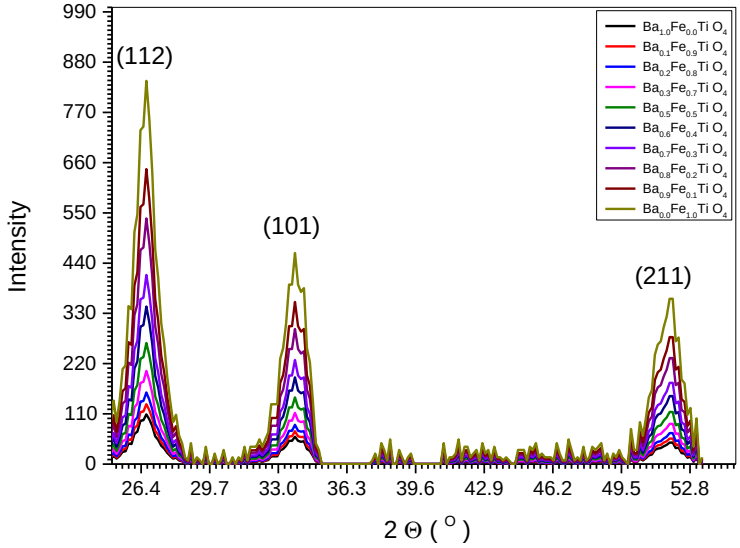

Fig (1) XRD spectrum of all ($Ba_x Fe_{(1-x)} Ti O_4$) samples

Table (1) some crystallite lattice parameter (c- form , a,b,c, β,α, γ, density ,Xs(nm) and d – spacing) of ($Ba_x Fe_{(1-x)} Ti O_4$) (1, 0.1 ,0.2 ,0.3 ,0.5 ,0.6, 0.7,08 ,0.9 and 0) Molar.

Sample	a=b	C	α=β = γ	Average Lattices constant	Xs(nm)	d-spacing
$Ba_{0,0}Fe_{1.0}TiO_4$	4.7033	3.3056	90	4.7282	12.6	2.5861
$Ba_{0.1}Fe_{0.9}TiO_4$	4.7033	3.3056	90	4.7275	12.4	2.5860
$Ba_{0.2}Fe_{0.8}TiO_4$	4.7033	3.3056	90	4.7273	12.4	2.5859
$Ba_{0.3}Fe_{0.7}TiO_4$	4.7033	3.3056	90	4.7273	12.3	2.5858
$Ba_{0.5}Fe_{0.5}TiO_4$	4.7033	3.3056	90	4.7268	11.9	2.5856
$Ba_{0.6}Fe_{0.4}TiO_4$	4.7033	3.3056	90	4.7263	11.8	2.5455
$Ba_{0.7}Fe_{0.3}TiO_4$	4.7033	3.3056	90	4.7261	11.7	2.5433
$Ba_{0.8}Fe_{0.2}TiO_4$	4.7033	3.3056	90	4.7260	10.8	2.5432
$Ba_{0.9}Fe_{0.1}TiO_4$	4.7033	3.3056	90	4.7256	10.6	2.5431
$Ba_{10}Fe_{0.0}TiO_4$	4.7033	3.3056	90	4.6104	9.4	2.5430

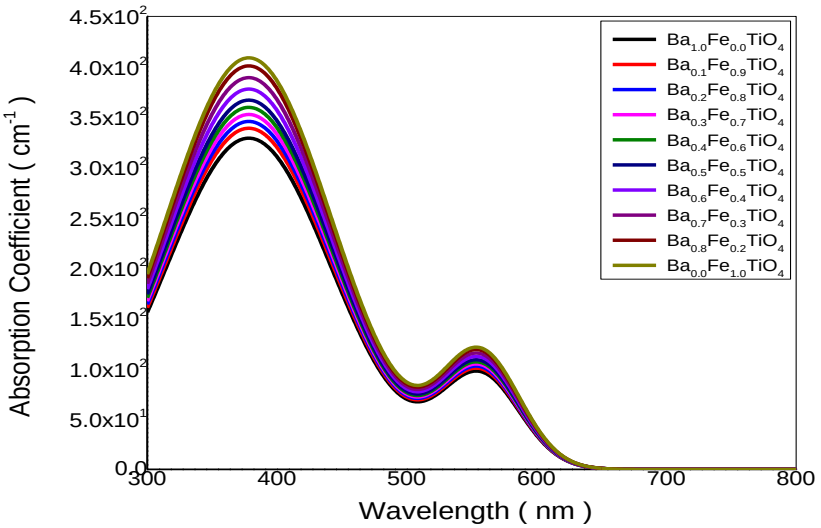

Fig (2) Absorption Coefficient spectrum of all ($Ba_x Fe_{(1-x)} Ti O_4$) samples

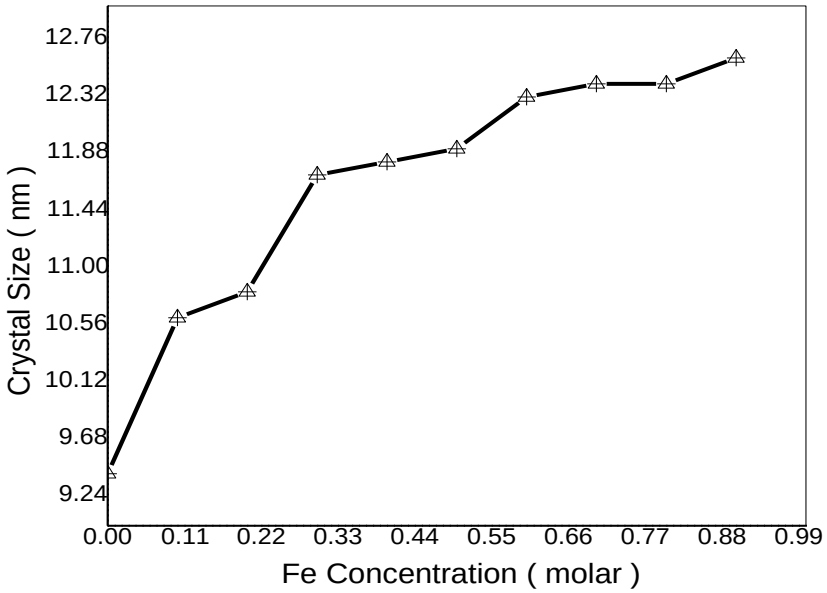

Fig (3) relationship between the Fe Concentration and Crystal Size
Of all ($Ba_x Fe_{(1-x)} Ti O_4$) sample

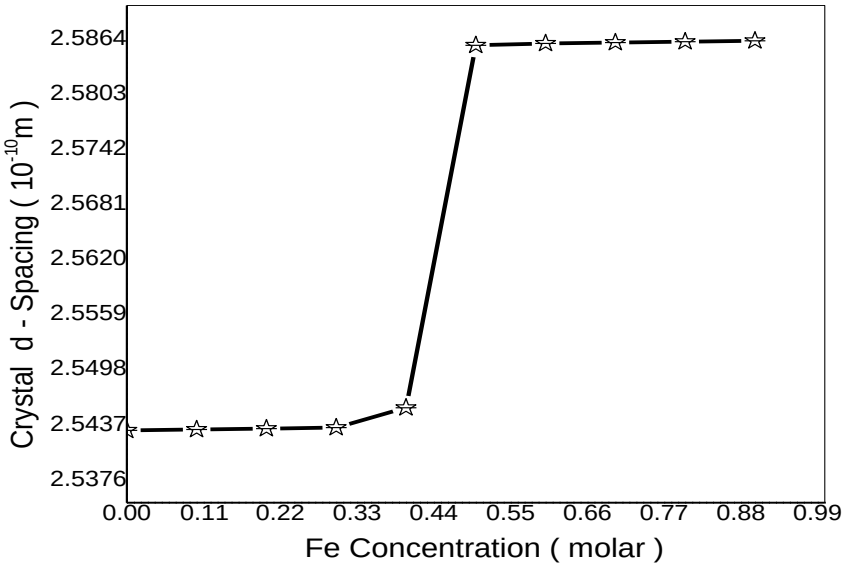

Fig (4) relationship between the Fe Concentration and Crystal d- Spacing
Of all ($Ba_x Fe_{(1-x)} Ti O_4$) sample

IV. Discussion

The compound ($Ba_xFe_{1-x}TiO_4$) (1, 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), fig (3) and fig(4). Figure (2) indicates that decreasing Fe concentration increases absorption coefficient and decrease the energy gap. Thus may be related to the effect of Fe on splitting of energy level. The energy given by

$$E_g = E_c - E_v = (E_{C0} - E_{VO}) - 2\Delta E \quad (1)$$
$$= (E_{C0}-E_{V0}) + 2BH \quad (2)$$
$$\Delta E = E_0 - BH \quad (3)$$

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 decreases of energy gap increases absorption and absorption coefficient as shown in figure (2). This may be attributed to the fact that decreasing the energy gap allows longer wavelength beside the shorter wavelengths to be absorbed by electron to move from the valence to the conduction band.

V. Conclusion:

Increasing Fe concentration increases crystal size and crystal spacing. The absorption coefficient decreases upon increasing Fe concentration and crystal size.

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