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Mathematical Simulation of Magnetic properties of Cu-Ti substituted Barium Hexaferrite

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Abstract: The parent hexaferrite $BaFe_{12}O_{19}$ is substituted by Cu^{2+} and Ti^{4+} ions by the conventional solid state diffusion method in three different concentrations and the magnetic properties are investigated. In this work a mathematical model is developed which gives the simulation of the experimental data in terms of mathematical equations so that the dependence of magnetic properties on various factors can be quantified. For this purpose the effect of concentration of Cu-Ti ions together and Fe ions, on the magnetic properties like saturation magnetization (M_s), coercivity (H_c) and Curie temperature (T_c) is used to represent the model.

Key words: Hexaferrites, Magnetic characterization, Mathematical model

Introduction:

Barium hexaferrite ($BaFe_{12}O_{19}$) or BaM is well studied hexagonal M-type ferrimagnetic material due to its number of applications in high density magnetic recording, electrical and electronic devices, transformers, etc.[1-6] Many researchers have studied the effect of substitution of Fe^{3+} ions with other trivalent metal ions like Mn^{3+} or combinations of divalent - tetravalent metal ions such as Zn^{2+}-Sn^{4+}, Co^{2+}-Sn^{4+}, Ni^{2+}-Zr^{4+}, Co^{2+}-Ti^{4+}, Mn^{2+}-Ti^{4+}, etc.[6]

The structural, magnetic, electrical and the dielectric properties of the substituted hexaferrites strongly depend on the electronic configuration of the substituted cations, their site preferences, concentration of the substituents as well as the methods of synthesis. Many authors investigated the properties for Cu^{2+}-Ti^{4+} substituted hexaferrites where Fe^{3+} ions are partly substituted. [7-9].

The magnetization (M) of BaM arises due to its magnetic structure which was first described by Gorter [10]. The structure of $BaFe_{12}O_{19}$ is built up by ten layers of oxygen ions which are formed by a close packing of cubic or hexagonal stacked layers alternately. The whole structure can be symbolically described as RSR*S*, where R* and S* blocks are built up by a rotation of 180º around the hexagonal *c*-axis [11].

Within the basic structure, the Fe^{3+} ions occupy five different interstitial sites. Three octahedral sites (2a, 12k and $4f_2$), one tetrahedral ($4f_1$) and one trigonal bipyramidal (2b) site. Three parallel (2a, 12k, 2b) and two antiparallel ($4f_1$, $4f_2$) sublattices are coupled through super exchange interactions through O^{2-} ions which form ferrimagnetic structure [11, 12]. Therefore each magnetic sublattice makes a specific contribution to the total magnetic moment and to the magnetocrystalline anisotropy of $BaFe_{12}O_{19}$.The crystallographic and magnetic properties of the five sublattices of M type hexaferrite are summarized in Table 1.

Table 1: Structural and magnetic parameters for the various cation sites of M type hexaferrite

Sublattice	Coordination	Block	Ions per molecule	Spin direction
12k	Octahedral	R-S	6	up
2a	Octahedral	S	1	up
2b	Bipyramidal	R	1	up
$4f_1$	Tetrahedral	S	2	down
$4f_2$	Octahedral	R	2	down

Experimental

The polycrystalline hexaferrites with composition $BaFe_{12-2x}Cu_xTi_xO_{19}$ (x = 1, 1.5, 2) were synthesized by the conventional ceramic technique using high purity Fe_2O_3 (Sigma – Aldrich), CuO, BaO and TiO_2 (all Merck). The structural and morphological properties of these samples were investigated with XRD (X-ray diffraction) and SEM (Scanning electron microscopy) respectively and described elsewhere [13] along with the detailed procedure of synthesis. In the present study the parent hexaferrite BaM is modified by partly substituting Fe^{3+} ions by a combination of Cu^{2+}-Ti^{4+} ions in three different concentrations. Cu^{2+} has magnetic moment $1\mu_B$ and is thus less magnetic in nature as compared to Fe^{3+} ions whose magnetic moment is $5\mu_B$. The variation of magnetization (*M)* with magnetic field (*H)* at room temperature gives the magnetic hysteresis from where the values of M_s, M_r, squareness ratio (SQR = M_s/M_r) H_c *and* T_c are calculated. The variation of *M* with *T* at constant field 1.2 T was carried out to find T_c. The results of this study are reported elsewhere [13].

In the present study the effect of substitution of Cu^{2+}-Ti^{4+} on magnetic properties of $BaFe_{12-2x}Cu_xTi_xO_{19}$ are quantified using mathematical simulation. XRD and SEM studies of these samples were carried out and the results were published elsewhere [13]. These results show that all the samples are single phase magnetoplumbite with hexagonal structure and the SEM study shows well formed grains separated by prominent grain boundaries.

2. Results and Discussion:

Mathematical simulation:

Artificial Neural Network (ANN) is a widely used tool for the quantitative analysis of the experimental data. Whenever a property is studied using any experimental technique, it is influenced by different factors like the constituents of the compounds under study, variation in their concentrations, temperature, dimensions of the equipment used for experimentation, environmental conditions, etc. These factors are called ‘cause’ and the property which is changing because of these ‘cause’ is called ‘effect’. Using these cause and effect some related mathematical equations are developed [14]. After solving these equations it may be concluded that which factor is more influential than the other and by how much quantity it is more effective than the others. Thus mathematical modeling may be considered as a mathematical proof of the experimental observations.

In this work a modest attempt has been made to develop a mathematical model which gives the simulation of the experimental data in terms of mathematical equations. In this regard the effect of concentration of Cu-Ti ions together (C) and Fe ions (F) on the magnetic properties like M_s, H_c and T_c is used to represent the model. The same principle can be used to extend the model using other substitutions and other properties.

Model for Cu-Ti substituted samples:

From the discussion of magnetic properties in the above mentioned sections it is observed that the concentration of Cu-Ti and Fe ions is one of the reasons to alter the magnetic parameters M_s, H_c and T_c of the compounds.

The selected causes and effects for the mathematical modeling are tabulated below.

Sr. No.	Sample	No. of atoms in the sample		M_s (emu/g)	H_c (emu)	T_c (°C)
		Cu-Ti (C)	Fe (F)			
1	C1	2	10	47.30	731.4	441
2	C1.5	3	9	29.73	91.58	316
3	C2	4	8	14.33	11.10	263

The mathematical equations for the model can be written as-

M_s = k $(C)^{x1}$ $(F)^{y1}$ ….. (1)

H_c = k $(C)^{x2}$ $(F)^{y2}$ ….. (2)

T_c = k $(C)^{x3}$ $(F)^{y3}$ ….. (3)

The values of the exponents x1, x2, x3 and y1, y2, y3 help to interpret the dependence of the properties on a particular cause. It can also be known by how much quantity one factor is influential over the others. These results are obtained quantitatively.

For the changes in magnetic properties several other factors like presence of other constituents, structural changes, environmental conditions, experimental factors, etc. these are all taken into account by the factor k. By reducing or eliminating these factors to the best possible extent the accuracy of the model can be increased. This would change the values of the exponents in the equations 4.2-4.4 and thus the quantitative influence of the causes can be found more accurately.

In the present case by solving equations 4.2-4.4 for various values of C, F and magnetic parameters, the values of the exponents can be found out. It is observed that

x1 = 1.2628, y1 = 9.2725, k = 1.053×10^{-8}

From (1),

$M_s = 1.053 \times 10^{-8} \times (C)^{1.2628} \times (F)^{9.2725}$ …… (4)

x2 = -1.2857, y2 = 14.7806, k = 2.9949×10^{-12}

From (2),

$H_c = 2.9949 \times 10^{-12} \times (C)^{-1.2857} \times (F)^{14.7806}$ …… (5)

x3 = -1.1371, y3 = 1.2127, k = 59.4359

From (2),

$T_c = 59.4359 \times (C)^{-1.1371} \times (F)^{1.2127}$ …… (6)

4.7. Inferences from the model:

1. The equations 4, 5 and 6 represent the quantitative influence of the substitution on various magnetic parameters. Due to the different ionic radii of Cu (0.70 Å), Ti (0.61 Å) and Fe (0.67 Å) the structural coordinates change which in turn may change the magnetic parameters.
2. In this model the factors C (concentration of Cu-Ti ions) and F (concentration of Fe ions) are cause which are responsible for changing M_s, H_c and T_c which are termed as effect.
3. It is observed from the model that F is more influential as compared to C and it is expected also because Fe^{3+} ions (magnetic moment $5\mu_B$) are replaced by Cu^{2+} ($1\mu_B$) and non magnetic Ti^{4+} ions.

4. The positive value of the exponent suggests that the particular cause increases the value of the effect and negative exponent indicates that the cause is inversely changing the magnetic parameter.

5. For saturation magnetization (M_s), the exponents x1 and y1 both are positive but concentration of Fe is more significant hence as F decreases, the value of M_s also decreases.

6. For coercivity (H_c) and Curie temperature (T_c), the respective exponents of C i.e. x2 and x3 are negative suggesting that as C increases, H_c and T_c both decrease. Whereas exponent of F i.e. y2 and y3 are positive. Thus as F decreases, H_c and T_c both decrease.

7. The value of k accounts for the other factors like temperature, dimensions of the experimental equipment, the other constituents of the compounds etc. which are remaining constant. Thus the value of k gives the influence of the other factors.

8. The experimental results match well with the mathematical equations.

The mathematical model thus includes all those factors affecting the property under study and thus may be helpful in deciding the conditions favorable and most suitable for the further study.

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