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**STRUCTURAL CHARACTERIZATION OF YTTRIUM-
EUROPIUM GARNET $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$**



Shesherao S. Jawale

Department of Electronics, Yeshwantrao Chavan
Mahavidyalaya, Tuljapur, Dist-Osmanabad,
Maharashtra, INDIA.

Corresponding author: drssjawalepatil@gmail.com

ABSTRACT:

The samples of $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system were prepared by using high purity oxides of Y_2O_3 , Eu_2O_3 , Fe_2O_3 and Al_2O_3 . X-ray diffraction patterns were recorded at room temperature using Philips X-ray diffract meter using $Cu-K\alpha$ radiation XRD Pattern were recorded in the 2θ range of 20° to 80° . X-ray diffraction data of the system $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ showed the system X-ray diffraction patterns were indexed and all the samples were found to have a cubic structure. The Values of theoretical and experimental lattice constant fairly agree with each other.

KEYWORDS: Yttrium iron garnet, $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$, cation distribution.

INTRODUCTION:

The compound with general formula $M_3T_5O_{12}$ (where M stands for lanthanide Sm-Lu and yttrium and T for Fe, Ge, Al etc.) are usually termed as garnet. These materials were first identified by Bertaut and Forrat [1] and independently by Geller and Gilleo [2].

Ferrite garnets are uncompensated anti-ferromagnetism and exhibit many interesting anomalies which shed light on the nature of anti-ferromagnetization and on the relationship between physical property and crystal structure.

The ferromagnetic oxide yttrium iron garnet (YIG) is an important material for a number of technical applications. Depending on the type of application, it is used in the form of bulk, single crystal, epitaxially grown thin film or polycrystalline sintered samples. These three forms are necessarily properties, e.g. resistivity, optical absorption, lattice constant and photo magnetic properties [3].

Yttrium iron garnet (YIG) is a microwave ferrite and in polycrystalline form has specific characteristics. Yttrium iron garnet in solid solution have become technologically significant for making devices, owing to their efficient for handling of microwave power [4]. It is well known that the microstructure of these materials depends on the microstructure of these materials depends on the initial powers and methods used in the synthesis of garnets. They can be prepared by not pressing [5], co-precipitation, hot spraying yttrium iron garnet show wide variety of interesting magnetic properties [7,8,9].

Thus, the study of electrical and magnetic properties of pure yttrium iron garnet and substituted yttrium iron garnet is important from the theoretical and application point of view. The magnetic crystallographic properties of pure yttrium iron garnet and substituted yttrium iron garnet have been studied extensively [7,10,11].

To our knowledge very few reports of the structural, electrical and magnetic properties of substituted yttrium iron garnet are available in the literature [12,13,14].

Patuthenet [15] has reported magnetic data for Europium iron garnet. Similarly, magnetic properties of pure yttrium iron garnet are reported in the literature [16]. In the work reported earlier [17] substitution of other trivalent ions for Fe^{3+} in $Y_3Fe_5O_{12}$ was investigated. The results of this work indicated that among non-magnetic ions the larger ones prefer the tetrahedral site; larger ones prefer the tetrahedral site, whereas smaller ones prefer the octahedral site. The magnetic and electrical properties of mixed yttrium Europium garnet substituted with non-magnetic Al^{3+} ions have not been studied to best of our knowledge.

In the present work, systematic investigations of structural properties of yttrium-europium garnet ($Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$) were carried out.

EXPERIMENTAL:

The sample of the series $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ were prepared using high purity oxides of Y_2O_3 , Eu_2O_3 , Fe_2O_3 and Al_2O_3 . Appropriate quantities of the constituents were mixed thoroughly in agate pestle mortar for 4 hours. The resulting powders were ground for 2 hours. The powder were ground and preheated at $1100^\circ C$ at 24 hours. Then it was further mixed and ground cylindrical pellets and fired at $1400^\circ C$ for 24 hours. Finally, the pellets were cooled to room temperature at the rate of $2^\circ C$ per minute.

X-ray diffraction patterns were recorded at room temperature using Philips X-ray diffract meter using $Cu-K\alpha$ radiation XRD Pattern were recorded in the 2θ range of 20° to 80° .

RESULT AND DISCUSSION:

The room temperature X-ray diffraction patterns are shown in fig. 5.1 and fig. 5.2. X-ray diffraction data of the system $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ showed the system X-ray diffraction patterns were indexed and all the samples were found to have a cubic structure. Using miller indices of the XRD peak, inter-planer spacing ‘d’ values of all the samples were determined and represented in Table 5.1.

Table 5.1: Miller indices (hkl) and inter-planer spacing (d) for $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system ($x = 0.0$ to 1.0)

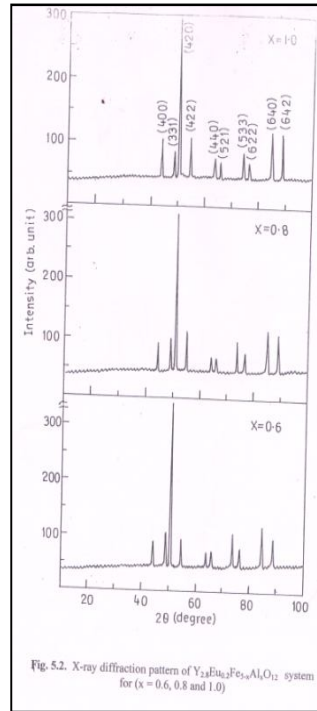
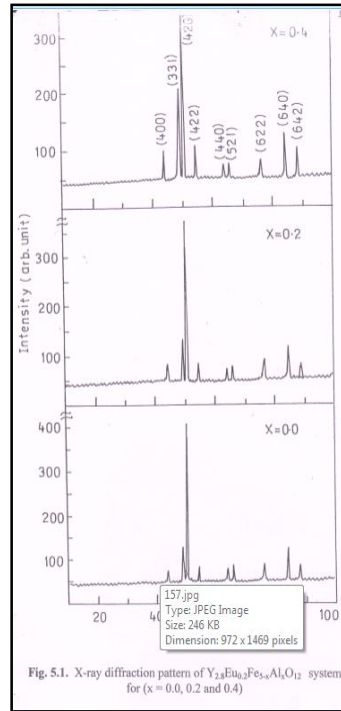
Plane (hkl)	Inter-planer spacing ‘d’ (Å)					
	X = 0.0	X = 0.2	X = 0.4	X = 0.6	X = 0.8	X = 1.0
(400)	4.001	4.004	4.018	4.002	4.038	4.043
(331)	4.400	4.433	4.437	4.441	4.453	4.454
(420)	4.469	4.478	4.489	4.502	4.513	4.510
(422)	4.899	4.908	4.922	4.936	4.942	4.943
(440)	5.699	5.698	5.705	5.709	5.704	5.710
(622)	6.640	6.643	6.649	6.656	6.678	6.670
(640)	7.223	7.229	7.243	7.263	7.207	7.282
(642)	7.491	7.504	7.517	7.539	7.554	7.500

The lattice constant of all the samples were determined from X-ray data and the values are listed in Table 5.2. The lattice constant values are in good agreement with the results of other garnet system [18, 19].

Table 5.2: Lattice constant (a) and particle size (t) for $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system $X = 0.0$ to 1.0)

Composition ‘x’	Lattice constant ‘a’ (Å)		Particle size ‘t’ (Å)
	Obs.	The	
0.0	12.340	12.329	150
0.2	12.325	12.310	151
0.4	12.308	12.291	151
0.6	12.290	12.270	151
0.8	12.251	12.250	151
1.0	12.248	12.231	151

Fig 5.3 depicts the variation of lattice constant with Al substitution. It is evident from fig. 5.3 that lattice constant decreases linearly with Al substitution. This behaviour of lattice constant can be explained on the basis of difference in ionic radii of the constituents ions.



In the present of $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ the magnetic Fe^{3+} ions are replaced by non-magnetic Al^{3+} ions. Since ionic radii of Al^{3+} (0.51\AA) ions is smaller than that of Fe^{3+} (0.64\AA), the lattice constant decreases with Al substitution, similar behaviour of lattice constant with composition was reported in the literature [20].

The particle diameter of all the samples was calculated using the following formula,

$$t = \frac{0. \lambda}{B \cos \theta_B} \tag{5.1}$$

Where notation have their usual meaning.

The X-ray density of the all the samples of the series were calculated using the relation [21].

$$d_x = \frac{ZM}{NV} \text{ gm/cm}^3 \tag{5.2}$$

Where,

Z: is the number of molecule per unit cell, M: is the molecular weight, N Avogadro’s number and V is the volume of the unit cell.

The values of X-ray density obtained by using the above the above relation are presented in Table 5.3. it is observed from table 5.3 that X-ray density decreases with Al^{3+} substitution.

Table 5.3: Molecular weight (M), X-ray density (d_x), bulk density (d) and porosity for $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system X = 0.0 to 1.0

Composition 'x'	Mo1. wt 'M' (gm)	X-ray density 'd' (g/cm ³)	Bulk density 'd' (g/cm ³)	Porosity 'P' %
0.0	751	5.303	5.113	2.270
0.2	745	5.282	5.024	4.868
0.4	739	5.263	5.236	0.516
0.6	733	5.245	4.542	13.40
0.8	727	5.231	4.676	10.61
1.0	722	5.215	4.899	6.050

The fig. 5.4 shows variation of X-ray density with aluminum content X. is seen from fig. 5.4 that X-ray density decreases with the fact that the decrease in mass overtakes decrease in lattice constant.

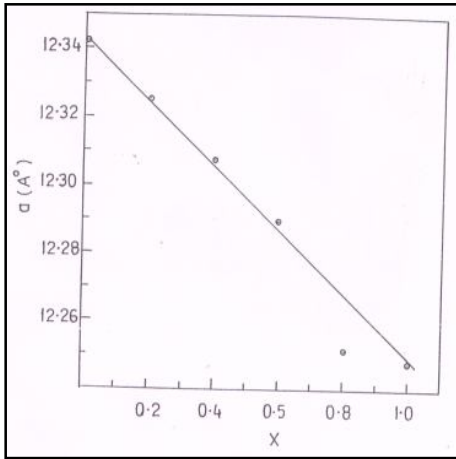


Fig.5.3. Variation of lattice 'a' with composition (x= 0.0.1.0) for of $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system

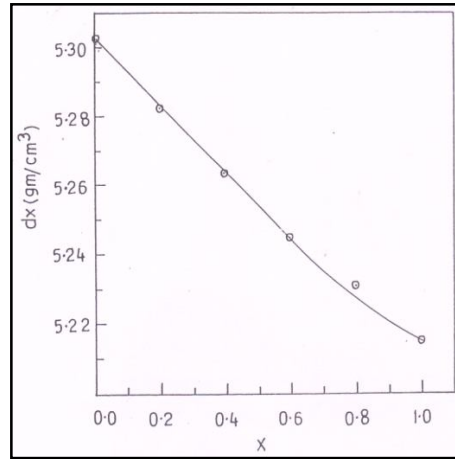


Fig.5.4. Variation of X-ray 'dx' with composition 'x' (X= 0.0.1.0) for of $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ system

The bulk density of all the samples was calculated knowing the mass and volume of the pellet. The values of the bulk density are presented in Table 5.3.

The percentage porosity (P) of all the samples were calculated using the following relation and the values are given in Table 5.3.

$$P = \left(1 - \frac{d}{d_x}\right) \times 100 \% \quad (5.3)$$

Where, d is bulk density and d_x is X-ray density

CATION DISTRIBUTION

The magnetic properties of ferrites (spinel, garnet and hexaferrite) depend upon method of preparation and the distribution of cations among the available sites. It is very understand the properties of ferrites.

Yttrium iron garnet (YIG) belongs to the space group o_h^{10} ($1A3_d$) and has seven non site and four octahedral (a) site in it. Normally, in garnet cations are distributed at three available sub lattices namely dodecahedral (c) octahedral (a) and tetrahedral (d).

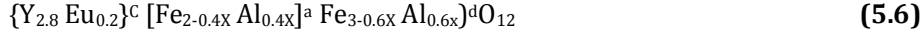
In garnet, the net magnetic moment (in Bohr magneto per unit formula) is given by,

$$M = 3m_c - 5\mu_B \quad (5.4)$$

In general, the Cation distribution of yttrium iron garnet is expressed as,



Comparing the site preference energy of the constituent ions and assuming that yttrium and europium ions occupy dodecahedral C-sites, the approximate Cation distribution of the present garnet system $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ can be written as,



The average ionic radius in the cations sites can be obtained using the following equations,

$$r_d = [x(Fe^{3+}).r(Fe^{3+})] \text{ (for d site)} \quad (5.7)$$

$$r_a = \frac{1}{2}[(XFe^{3+}).r(Fe^{3+}) + x(Fe^{2+})] \text{ (for a site)} \quad (5.8)$$

$$r_c = [x(Y^{3+}).r(Y^{3+}) + X(Fe^{3+}).r(Fe^{2+})] \text{ (for d site)} \quad (5.9)$$

Where, x and r represents concentration and ionic radius above equations (5.7, 5.8 and 5.9), considering the ionic radii of yttrium Y^{3+} as (0.89Å), Europium Eu^{3+} as (0.95Å), aluminum Al^{3+} (0.51 Å) and ferric (Fe^{3+}) as (0.64 Å) and the Cation distribution formula given by eqⁿ 5.6, the radius of dodecahedral (c), octahedral (a) and tetrahedral (d) were calculated and the values are summarized in Table 5.4.

Table 5.4: Ionic radii of dodecahedral (r_c), octahedral (r_a), tetrahedral (r_d) sites and average radius for system $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ ($X = 0.0$ to 1.0)

Composition 'x'	r_c (Å)	r_a (Å)	r_d (Å)	Average radius (Å)
0.0	0.894	0.640	0.640	0.725
0.2	0.894	0.635	0.635	0.721
0.4	0.894	0.630	0.630	0.718
0.6	0.894	0.624	0.624	0.714
0.8	0.894	0.619	0.619	0.711
1.0	0.894	0.614	0.614	0.707

The theoretical lattice constant of all the samples were also estimated using the formula [22],

$$a_{th} = b_1 + b_2r_c + b_3r_d + b_4r_a + b_5r_c r_d + b_6r_c r_6 \quad (5.10)$$

The value of theoretically obtained lattice constant is given in the Table 5.1. The Values of theoretical and experimental lattice constant fairly agree with each other.

CONCLUSION:

1. Analysis of X-ray diffraction pattern indicates that all the samples possess single phase cubic garnet structure.
2. Lattice constant 'a' obtained from XRD data decreases with the increase in Al substitution.
3. Cation distribution data presented for the garnet system $Y_{2.8}Eu_{0.2}Fe_{5-x}Al_xO_{12}$ is in agreement with our earlier work.

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