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Effect of Fuel to Oxidizer Ratio (F/O) on $YFeO_3$ Phase Formation Using Glycine Fuel during Solution Combustion Process

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Abstract— **In this work nano crystalline YFeO3 powders were prepared by solution combustion process using yttrium nitrate hexahydrate Y(NO3)3.6H2O), ferric nitrate nonahydrate (Fe(NO3)3.9H2O) as oxidizers, glycine (H2NCH2C00H) as fuel. The effect of fuel to oxidizer ratio (F/O) on YFeO3 phase formation was investigated. The prepared samples were characterized by X-ray diffraction (XRD) for phase analysis. The experimental results revealed that the formation of pure crystalline phase of yttrium ferrite was confirmed for fuel rich samples with crystallite size 30-45 nm and fuel lean samples show amorphous phase when comparing the obtained peaks of XRD pattern with the peaks of standard XRD pattern of JCPDS card number 39-1489**

Index Terms— Combustion, glycine, $YFeO_3$.

I. INTRODUCTION

Perovskite ABO_3 series nanomaterials, one of the most attractive and interesting mixed oxides, has been used as functional material in many fields due to their unique properties, such as electrical, magnetic, semiconducting, catalytic and optical properties and its used in gas sensors, data storage devices, environmental monitoring applications and catalysis [1-2].

Yttrium ortho-ferrite($YFeO_3$), is one of rare earth iron perovskites. $YFeO_3$ based catalysts have been explored for photo catalytic oxidation of organic dyes and exhibit higher visible-light photo-catalytic activity [3]. $YFeO_3$ has been found to be ferromagnetic, which gives a possibility for recovery of $YFeO_3$ with an external magnet in practical applications. Nano-powders are attracting the scientists, researchers, industrial people due to their unique properties compared with their bulk counterpart due to high surface area [4]. Hence synthesis of nanopowders has become necessary to get required unique properties

Up to now, various approaches have been applied to prepare perovskite $YFeO_3$, such as sol-gel [5-6], solid-state route [7-8], thermal decomposition [9], microwave [10] by using different chemical precursors and also by using Solution combustion synthesis [1-4], Among the various synthetic routes, solution combustion synthesis has been regarded as one of effective and economic approaches to its convenient processing, simple experimental setup, significant saving in time and energy and homogeneous products. However, solution combustion synthesis (SCS) of well-dispersed nano crystalline particles faces two difficulties of inhibiting particulate agglomeration and promoting phase formation. Considering the situation, many attempts have been made to prevent resultant particles from agglomerating and sintering by choosing fuel and adjusting fuel-to-oxidizer ratio [11-14].. Few groups reported the synthesis of $YFeO_3$ by solution combustion process by using glycine fuel .Till now no report has been made of studying the effect of fuel to oxidizer ratio on $YFeO_3$ phase formation.

In this work, the effect of fuel to oxidizer ratio (F/O) on the $YFeO_3$ phase formation was studied by using the glycine fuel with varying (F/O) of = 0.5, 0.75, 1, 1.25, 1.5 using yttrium nitrate hexahydrate $Y(NO_3)_2.6H_2O$), ferric nitrate nonahydrate $(Fe(NO_3)_3.9H_2O)$ metal nitrates as oxidizers.

II. EXPERIMENTAL DETAILS

A. Raw materials used

Yttrium nitrate hexa-hydrate $(Y(NO_3)_2.6H_2O)$. (Universal laboratories), Ferric nitrate Nona-hydrate $(Fe(NO_3)_3.9H_2O)$, (Universal laboratories), glycine (H_2NCH_2C00H) (Alchem).

B. Solution Combustion Synthesis of $YFeO_3$

3.83gm of yttrium nitrate hexa-hydrate and 4.04gm of ferric nitrate nona-hydrate were weighed on an electronic balance. Weighed yttrium nitrate and of ferric nitrate were dissolved in minimum quantity of distilled water with varying mass of glycine fuel as shown in the Table 1 for respective F/O composition. This mixture of chemicals was taken in a crucible bowl and rotated continuously till the dissolution of chemical, The chemical mixture was stirred using magnetic stirrer to ensure complete dissolution. During magnetic stirring process the chemical will be dissolved and the fuel can homogeneously mixed with all the metal nitrates in the mixture. The stirred solution was introduced into a furnace maintained at a temperature of 500^o C. Initially the solution boils and undergoes dehydration followed by decompositions of nitrates and fuel with evolution of gasses NH_3 and NO_X HCNO ,these gases mixing hypergolically give the gaseous combustion with exothermic reaction producing huge amount of energy and gases such as CO_2, H_2O, and N_2 with desired solid nano powders of product. This process was continued for the other volume of chemical mixtures. The same process will be carried out for the other mixture of chemicals also i.e, 3.83gm of yttrium nitrate, 4.04gm of ferric nitrate with effect of fuel to oxidizing ratio 0.5, 0.75, 1.25, 1.5 of glycine and The obtained product was brown in color. The synthesized powder were characterized by XRD for phase analysis and crystallite size determination. The combustion reaction

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characteristics and the combustion details like expected product, yield obtained , amount of chemicals taken and moles of chemical precursor and number of moles of fuel taken are shown in Table I. The combustion details like nature of combustion, time ,color of the flame, flame type, are shown in Table II.

All obtained powders were characterized by XRD. Under the equilibrium conditions the reaction equations in these fuel-nitrate systems for preparation of $YFeO_3$ of F/O = 0.5, 0.75, 1.0, 1.25, 1.5 respectively can be represented as below.

$$Y(NO_3)_3.6H_2O+Fe(NO_3)_3.9H_2O+1.66CH_2NH_2COOH \longrightarrow YFeO_3+(3.83)N_2+(3.32)CO_2+(19.15)H_2O \quad (1)$$

$$Y(NO_3)_3.6H_2O+Fe(NO_3)_3.9H_2O+2.5CH_2NH_2COOH \longrightarrow YFeO_3+(4.25)N_2+(5)CO_2+(21.25)H_2O \quad (2)$$

$$Y(NO_3)_3.6H_2O+Fe(NO_3)_3.9H_2O+3.33CH_2NH_2COOH \longrightarrow YFeO_3+(4.665)N_2+(6.66)CO_2+(23.325)H_2O \quad (3)$$

$$Y(NO_3)_3.6H_2O+Fe(NO_3)_3.9H_2O+4.166CH_2NH_2COOH \longrightarrow YFeO_3+(5.083)\ N_2+(8.332)CO_2+(25.415)H_2O \quad (4)$$

$$Y(NO_3)_3.6H_2O+Fe(NO_3)_3.9H_2O+5CH_2NH_2COOH \longrightarrow YFeO_3+(5.5)N_2+(10)CO_2+(27.5)H_2O \quad (5)$$

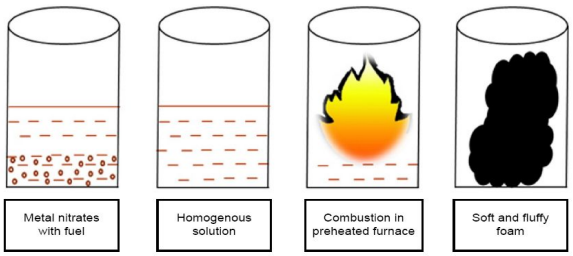

Figure 1. Solution combustion steps

C. Phase analysis of powders

Phase analysis of ceramic powder can be done by using D8-Advance-Bruker X-ray diffractometer machine with Cu-K_α (wavelength of Cu-K_α (λ) ~1.5406 Å) radiations for all the measurements. Ni filter was used to attenuate K_β lines. The crystallite sizes of the powders has been calculated form the XRD pattern using Scherer formula.

$$d = K \lambda / \beta \cos\theta \quad (6)$$

where, β_θ is the full width at half maximum (FWHM) of diffracted peaks in degrees,
d stands for the liner dimension of particles in meters,
θ refers to Bragg's angle in degrees
K' is the shape factor, generally known as a numerical constant and evaluated as 0.93 and depends on shape of crystallites.

Table.1 Amount of glycine fuel and oxidizers, used for the combustion reaction to produce $YFeO_3$

SNo	F/O Ratio	$Y(NO_3)_3.6H_2O$ in (gm)	$(Fe(NO_3)_3.9H_2O$ in (gm)	Fuel Glycine in (gm)	Expected in (gm)	Obtained in (gm)
01	0.5	3.83	4.04	1.24	1.93	1.39
02	0.75	3.83	4.04	1.87	1.93	1.46
03	1	3.83	4.04	2.49	1.93	1.59
04	1..25	3.83	4.04	3.12	1.93	1.62
05	1.5	3.83	4.04	3.75	1.93	1.73

Table 2 Characteristics of the combustion reaction of various F/O using glycine fuel to produce $YFeO_3$

Sl No	Sample code	F/ O Ratio	Sample	Glycine fuel in gm	Color	Reaction	Combustion time
1	PSK01	0.5	3.83gm Yttrium nitrate + 4.04gm ferric nitrate	1.24	Brown	No Flame and Foam formation	7.02 min
2	PSK02	0.75	3.83gm Yttrium nitrate + 4.04gm ferric nitrate	1.87	Brown	Flame and foam formation	7.12 min
3	PSK03	1	3.83gm Yttrium nitrate + 4.04gm ferric nitrate	2.49	Brown	Flame and Foam formation	7.19 min
4	PSK04	1.25	3.83gm Yttrium nitrate + 4.04gm ferric nitrate	3.12	Dark brown	Flame but no foam formation	7.36 min
5	PSK05	1.5	3.83gm Yttrium nitrate + 4.04gm ferric nitrate	3.75	Dark brown	flame and foam formation	7.20 min

III. RESULT AND DISCUSSION

A. Phase analysis of powders prepared by variation of fuel/oxidizer ratio

Figure 2-6 show XRD patterns of the as synthesized powder prepared by solution combustion synthesis using glycine as fuel at 500°C for all compositions of various F/O . Figure 7 shows the combined XRD patterns of all samples. All the peaks in the XRD patterns of F/O =1, 1.25, 1.5 of Figure4-6 respectively are very sharp showing the well crystalline behavior of the heat treated powders. The formation of phase pure crystalline $YFeO_3$ is confirmed by comparing the peaks with standard peaks of JCPDS card no 39-1489. The identified phases present in the patterns of $YFeO_3$ are of Orthorhombic pervoskite. However, small impurity phases were detected in the XRD pattern of $YFeO_3$ powder prepared using glycine as a fuel for these fuel rich composition. The XRD patterns of the compositions F/O=0.5, 0.75. of Figures 2-3 from the XRD data, it was found that amorphous to partial crystallization of $YFeO_3$ could be achieved by solution combustion synthesis process using less glycine as fuel(fuel lean). The intensities of peaks are broad .

The intensity of the peak varies with change in F/O ratio . Intensity increases as the F/O ratio increases and reaches highest at the stoichiometric ratio F/O=1 and further decreases as F/O ratio increases. The intensity is parabolic ally related with the F/O.

This change in the intensity with the F/O during combustion is due to variation in exothermicity. The gradual decrease of exothermicity as increase in the F/O ratio after stoichiometric (fuel rich region) is due to incomplete combustion reaction occurring via unavailability of oxygen molecules for complete combustion, thus adiabatic flame temperature decreases and this leads to formation of nano powders of crystallite size 2, 7, 45, 41, 33 nm respectively for the F/O = 0.5, 0.75, 1.0, 1.25, 1.5 compositions. The variation of crystallite size is parabolically with the F/O due to the reasons as explained for intensity of peaks.

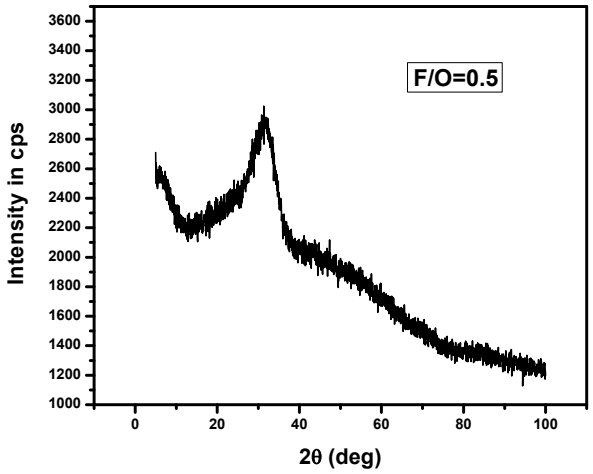

Figure 2. XRD pattern of F/O = 0.5

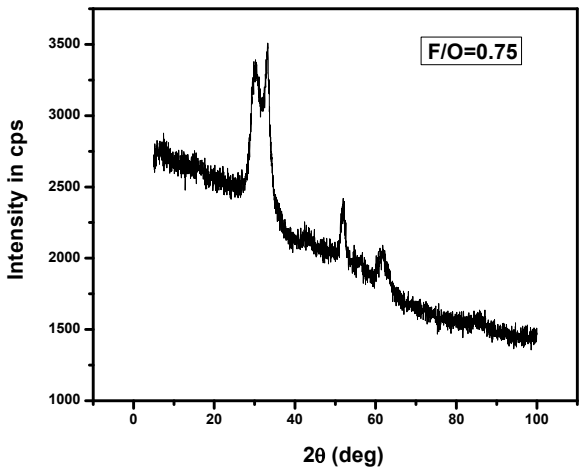

Figure 3. XRD pattern of F/O = 0.75

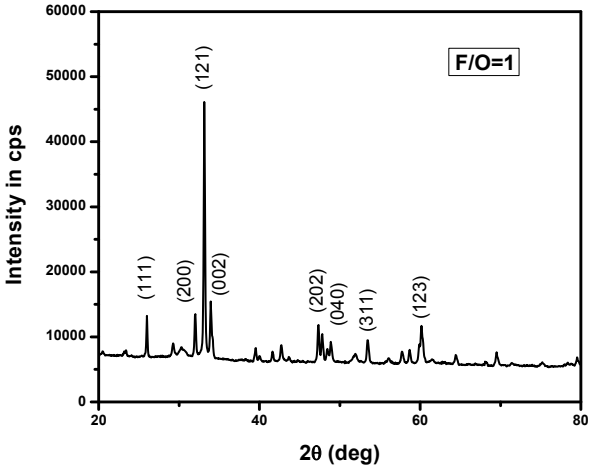

Figure 4. XRD pattern of F/O = 1

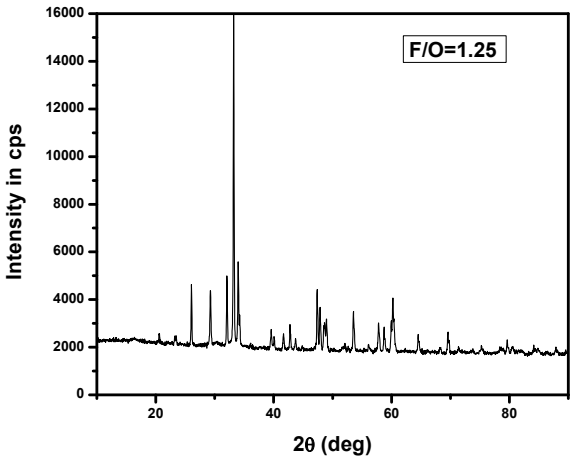

Figure 5. XRD pattern of F/O = 1.25

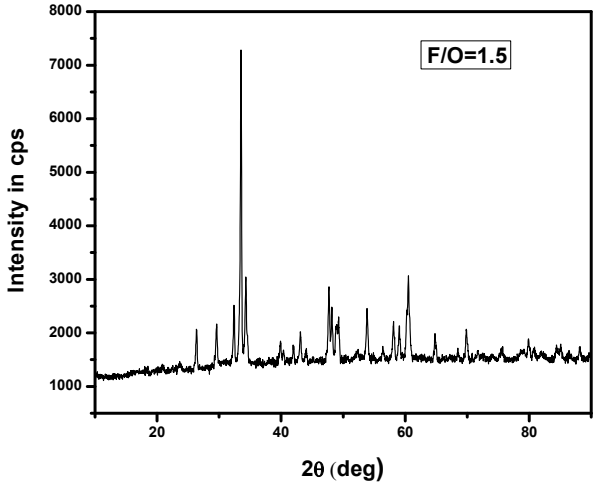

Figure 6. XRD pattern of F/O = 1.5

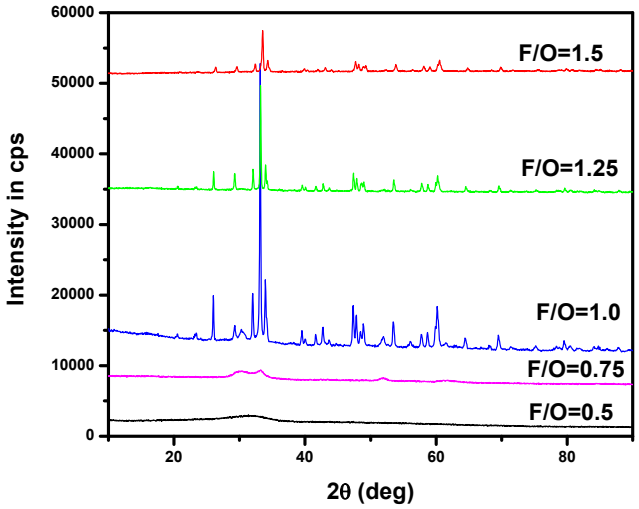

Figure 7. Total XRD pattern of F/O.

CONCLUSION

Phase pure $YFeO_3$ nanopowders were prepared by solution combustion method for stoichiometric composition and for excess glycine fuel (fuel rich) for the first time. The effect of fuel to oxidizer ratio on phase formation of $YFeO_3$ is carried out for the first time. Increase in F/O ratio increases the crystallinity. Fuel lean compositions of F/O ratio 0.5,0.75 show low crystallinity. The crystallite size is parabolically related to the F/O ratio.

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