International Journal of Research
Available at https://journals.pen2print.org/index.php/ijr/
e-ISSN: 2348-6848
p-ISSN: 2348-795X
Volume 06 Issue 09
August 2019

Study on Structural Properties of Ferrite Oxide (Fe_2O_3) Powder by Using XRD Method

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Abstract:

In this paper, Ferrite Oxide was used as the starting material. Crystal structure of the Fe_2O_3 sample was ascertained using X-ray diffraction (XRD) method. XRD Studies were carried out to undertaken the crystalline phase assignment, crystallographic orientation, lattice parameter of Fe_2O_3 powder. The lattice parameters were calculated with planer spacing formula by using characteristic peaks. These results were compared with standard profile.

Keywords

Ferrite Oxide Fe_2O_3, X-ray diffraction (XRD)

Introduction

A ferrite is a type of ceramic compound composed of iron oxide (Fe_2O_3) combined chemically with one or more additional metallic elements. Ferrites can be divided into two families based on their magnetic coercively, hard ferrite and soft ferrite. The crystalline state of solids is characterized by regular or periodic arrangement of atoms or molecules. The non-crystalline or amorphous solids are characterized by the completely random arrangement of atoms or molecules.

Iron Oxides (Fe_2O_3) are produced from ferrous, sulfate by heat soaking, removal of water, decomposition, washing, filtration, drying and grinding. They are produced in either anhydrous or hydrated forms. Their range of hues includes yellows, reds, browns and blacks. Iron oxide has been widely studied because of its nontoxicity, low cost, high stability under ambient conditions, and multi-functionality. Iron oxide had been intensively investigated for applications in lithium-ion batteries, sensors, catalysts and magnetic device.

X-ray crystallography can be used to determine the structure of the identified material i.e, how the atoms pack together in the crystalline state and what the interatomic distance and angle are etc. X-ray diffraction is one of the most important characterization tools used in solid state chemistry and materials science. The diffraction pattern obtained on a photographic film consisted of a series of dark spots arranged in a definite order. Such a pattern is called the Laue's pattern and reflects the symmetry of the crystal.

The dominant effect of X-ray that occurs when an incident beam of monochromatic X-rays interacts with a target material is scattering of those X-rays from atoms within the target material.

Experimental Procedure and Method

The purities of the starting materials, shown in the following figure, have been investigated with X-ray Diffraction Analysis. The phase and purity of the raw materials were checked by XRD, in Yangon Universities Researched Centre, to confirm these samples are pure or not.

Figure: Starting Material (Fe_2O_3)

A typical X-ray diffraction pattern is shown in below figure. The pattern consists of a series of peaks. The peak intensity is plotted on the y axis and the measured diffraction angle, 2θ, along the x-axis. The peaks are also called reflections.

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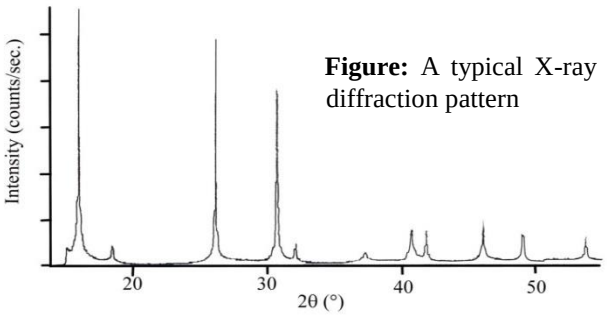

Figure: A typical X-ray diffraction pattern

Crystal Structure Determination

A typical example of indexing diffraction patterns obtained from materials with a Hexagonal structure is presented here. The procedure is the same for a metal, a semiconductor, or a ceramic. The hexagonal unit cell is characterized by lattice parameters ' a 'and 'c'. It can be obtained from the equation.

$$\frac{1}{d^2} = \frac{4}{3}\left[\frac{h^2+hk+k^2}{a^2}\right] + \frac{l^2}{c^2} \quad \ldots\ldots\ldots \quad (1)$$

Where, d = inter-planar spacing

(hkl) = Miller indices

a = lattice constant (a = b ≠ c)

n λ = 2d sin θ (Bragg's Law)

λ = 2d sin θ (first reflection)

$$d = \frac{\lambda}{2\sin\theta} \quad \ldots\ldots\ldots (2)$$

$$d^2 = \frac{\lambda^2}{4\sin^2\theta} \quad \ldots\ldots\ldots (3)$$

$$\frac{1}{d^2} = \frac{4\sin^2\theta}{\lambda^2} = \frac{4}{3}\left[\frac{h^2+hk+k^2}{a^2}\right] + \frac{l^2}{c^2} \quad \ldots\ldots\ldots (4)$$

$$\sin^2\theta = \left(\frac{\lambda^2}{4}\right)\left[\frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2}\right] \quad \ldots\ldots\ldots (5)$$

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)\left[\frac{4}{3}(h^2+hk+k^2) + \frac{l^2}{(c/a)^2}\right] \quad \ldots\ldots\ldots (6)$$

XRD Characteristics Measurement

Two approaches can be used to calculate the lattice parameters (' a ' and 'c'). First, ' a ' can be calculated by looking for reflections of the type hk0. When we substitute l = 0 and equation (6).

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)\left[\frac{4}{3}(h^2+hk+k^2)\right] \quad \ldots\ldots\ldots (7)$$

The lattice parameter ' a ' can be calculated from equation (7).

$$a^2 = \left(\frac{\lambda^2}{3\sin^2\theta}\right)(h^2+hk+k^2) \quad \ldots\ldots\ldots (8)$$

$$a = \left(\frac{\lambda}{\sqrt{3}\sin\theta}\right)\sqrt{h^2+hk+k^2} \quad \ldots\ldots\ldots (9)$$

Once the value of ' a ' is known 'c' can be calculated since the value of c/ a is known. Alternatively, we can look for the ($00l$) type reflections and calculate 'c' from equation (6) reduces to

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)\left[\frac{l^2}{(c/a)^2}\right] \quad \ldots\ldots\ldots (10)$$

$$c^2 = \left(\frac{\lambda^2}{4\sin^2\theta}\right)l^2 \quad \ldots\ldots\ldots (11)$$

$$c = \left(\frac{\lambda}{2\sin\theta}\right)l \quad \ldots\ldots\ldots (12)$$

The X-ray diffraction pattern of Ferrite Oxide recorded with CuK_α (λ=0.154056 nm) radiation is presented in the below figure. Six peaks exist in the diffraction pattern, and the 2θ values for these peaks. The $\sin^2\theta$ values have been calculated and determined the lattice parameter of Ferrite Oxide.

RESULTS AND DISCUSSIONS

The phase and purity of the raw materials (Fe_2O_3)

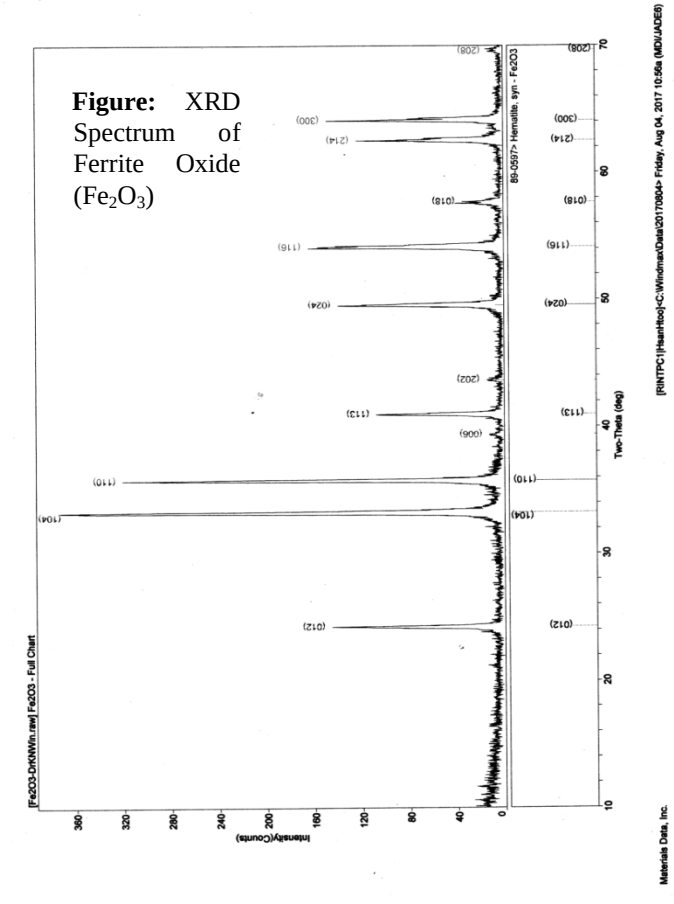

Figure: XRD Spectrum of Ferrite Oxide (Fe_2O_3)

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were checked by XRD to confirm these samples are pure or not in Yangon Universities Researched Centre. The XRD spectrum of Fe_2O_3 is shown in the figure. The XRD data of Fe_2O_3 is tabulated in following table (2).

The lattice parameter for standard X-ray diffraction pattern of Hexagonal is calculated from equation (6). a can be calculated by looking for reflections of the type $h\ k\ 0$ from equation (9). Once the value of a is known, c can be calculated since the value of c/a is known. Then, we can look for the ($00l$) type reflections and calculate c from equation (12). By using c/a ratio, the lattice parameters of the other planes can be calculated from equation (6). The lattice parameters values were organized in the table (1). After that, these theoretical results are compared with the experimental results that are measured by XRD method in Table (3).

Table (1): Work Table for Ferrite Oxide (Fe_2O_3) λ = 0.154056 nm

Peak	2θ(°)	$\sin^2\theta$	hk$l$	a (nm)	c (nm)
1	33.231	0.0818	104	0.5017	1.3700
2	35.759	0.0943	110	0.5018	-
3	39.330	0.1132	006	-	.3734
4	40.957	0.1224	113	0.5021	1.3740
5	49.548	0.1756	024	0.5024	1.3749
6	54.121	0.2069	116	0.5025	1.3753

Average value of a = 0.5021 nm

Average value of c = 1.3735 nm

Average value of c/a = 2.7355

Table (2): Lattice Parameters of Experimental Result for Fe_2O_3

Peak	2θ(°)	d (Å)	hk$l$	a (nm)	c (nm)
1	33.231	2.6938	104	0.5012	1.3742
2	35.759	2.5089	110	0.5018	-
3	39.330	2.2890	006	-	1.3734
4	40.957	2.2017	113	0.5052	1.3479
5	49.548	1.8382	024	0.5024	1.3749
6	54.121	1.6932	116	0.5025	1.3753

Average value of a = 0.5026 nm

Average value of c = 1.3691 nm

Average value of c/a = 2.7240

Table (3) Lattice Parameters of Theoretical and Experimental Results

Peak	hk$l$	Theoretical		Experimental	
		a(nm)	c(nm)	a (nm)	c(nm)
1	104	0.5017	1.3700	0.5012	1.3742
2	110	0.5018	-	0.5018	-
3	006	-	.3734	-	1.3734
4	113	0.5021	1.3740	0.5052	1.3479
5	024	0.5024	1.3749	0.5024	1.3749
6	116	0.5025	1.3753	0.5025	1.3753
Average value		0.5021	1.3735	0.5026	1.3691

Conclusion

In this work, the Ferrite Oxide (Fe_2O_3) sample was investigated to get lattice parameters by using powder X-ray diffraction method. According to theoretical results, the lattice parameter 'α' is as 0.5021 nm and 'c' is 1.3735 nm by X-ray method in Table (1) and the lattice constant of Fe_2O_3 'α' is 0.5026 nm and 'c' is 1.3691 nm in Table (2). Based on experimental data and theoretical calculation, the lattice parameters of Ferrite Oxide (Fe_2O_3) in theoretical results are nearly the same with experimental results shown in Table (3).

References

- http:// en.wikipedia. org/wiki/Ferrite Oxide
- Puri R. K &Babbar V. K (2003) "Solid State Physics and Electronics" (New Delhi :Ramnager)

Peak	2θ(°)	d (Å)	hk$l$	a (nm)	c (nm)