

Supplementary Materials

**EFFECT OF THERMAL-TREATMENT ON STRUCTURAL,
MÖSSBAUER AND MAGNETIC PROPERTIES OF ZN-NANOFERRITE**

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Details of the studied samples are as follows: synthesized 'dry gel' sample is labelled as DG, sample annealed at 600 °C / for 3 hours is labelled as ANN, and spark plasma sintered at 800 °C for 5 minutes is labelled as SPS.

Theoretical lattice parameter a_{th} , bond angles - $\theta_1, \theta_2, \theta_3, \theta_4, \theta_5$, Oxygen position parameter - u^{43m} were computed by cationic distribution, utilizing the following equations:

$$a_{th} = \frac{8}{3\sqrt{3}} \left[(r_A + R_0) + \sqrt{3}(r_B + R_0) \right] \quad (1)$$

where, r_A – A-site ionic radius, r_B – B-site ionic radius, R_0 – 0.138 nm is the radius of Oxygen ion.

$$u^{43m} = \frac{(r_A + R_0)}{(\sqrt{3} * a_{exp})} + \frac{1}{4} \quad (2)$$

where, R_0 – 0.138 nm is the radius of Oxygen ion, a_{exp} – experimental lattice parameter.

$$\left. \begin{aligned} \theta_1 &= \cos^{-1} \left[\frac{p^2 + q^2 - c^2}{2pq} \right], & \theta_2 &= \cos^{-1} \left[\frac{p^2 + r^2 - e^2}{2pr} \right], & \theta_3 &= \cos^{-1} \left[\frac{2p^2 - b^2}{2p^2} \right] \\ \theta_4 &= \cos^{-1} \left[\frac{p^2 + s^2 - f^2}{2ps} \right], & \theta_5 &= \cos^{-1} \left[\frac{r^2 + q^2 - d^2}{2rq} \right] \end{aligned} \right\} \quad (3)$$

The interionic distances between cations - b, c, d, e, f, and between cation and anion - p, q, r, s were estimated

from the a_{exp} and u^{43m} by using the following relations:

$$\left. \begin{aligned} b &= \frac{a_{exp} \cdot \sqrt{2}}{4}, & p &= a_{exp} \cdot \left(\frac{5}{8} - u^{43m} \right) \\ c &= \frac{a_{exp} \cdot \sqrt{11}}{8}, & q &= a_{exp} \cdot \sqrt{3} \cdot \left(u^{43m} - \frac{1}{4} \right) \\ d &= \frac{a_{exp} \cdot \sqrt{3}}{4}, & r &= a_{exp} \cdot \sqrt{11} \cdot \left(1 + u^{43m} \right) \\ e &= \frac{3a_{exp} \cdot \sqrt{3}}{8}, & s &= a_{exp} \cdot \sqrt{3} \cdot \left(\frac{u^{43m}}{3} + \frac{1}{8} \right) \\ f &= \frac{a_{exp} \cdot \sqrt{6}}{4} \end{aligned} \right\} \quad (4) \quad (5)$$

Where, a_{exp} – Experimental lattice parameter, and u^{43m} – Oxygen position parameter.

b, c, d, e, f - the distance between metal-metal cations (M_e - M_e), p, q, r, s – the distance between metal cations, and Oxygen anions (Me - O),.

Obtained cationic distribution was used to compute Neel magnetic moment ' n_N ' (in Bohr magneton ' μ_B '), is calculated by using the formula:

$$n_N = M_B - M_A \quad (6)$$

where M_A, M_B are respectively magnetic moments of A, B-site obtained by cationic distribution.

Theoretical magnetization at 0 K: $M_{s(th)}$, was obtained using following expression:

$$M_{s(th)} = [n_N \times \mu_B \times N_A] / m \quad (7)$$

where, n_N - Neel magnetic moment, μ_B - 0.9274×10^{-20} emu, N_A - Avogadro's number, m - molecular weight (g mol^{-1}).

Canting angle α_{Y-K} was computed using the equation :

$$\alpha_{Y-K} = \text{Cos}^{-1} \{ (n_{B(x)}^e + M_{A(x)}) / M_{B(x)} \} \quad (7)$$

where $M_{A(x)}$ and $M_{B(x)}$ are the magnetic moments expressed in Bohr magneton μ_B on A, B sites, and $n_{B(x)}^e$ is the experimental magnetic moment.

Magnetic dead layer thickness t was calculated by using the equation:

$$t = D_{W-H} / 6 [1 / (M_s / M_B)] \quad (8)$$

where, D_{W-H} – Williamson–Hall grain diameter, M_s – saturation magnetization, and M_B – bulk magnetization.

Anisotropy constant K_1 was calculated by using equation:

$$K_1 = [H_c \times M_s] / 0.96 \quad (9)$$

Where M_s – Saturation magnetization, H_c - coercivity

XRD patterns of the studied samples were Rietveld refined by software MAUD (*Material Analysis Using*

Diffraction) [1], and are shown as figure S1 (a to c). Peak position of $\alpha\text{-Fe}_2\text{O}_3$ phase is matched with ICDD No. 01-079-0007.

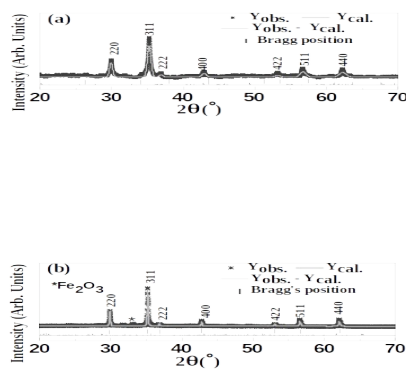


Figure S1: Reitveld refined XRD patterns of the studied (a) DG, (b) ANN, (c) SPS samples.

Table S1: Rietveld refined R-parameters (R_{wp} , R_p , R_{exp}), goodness of fit ($GOF = R_{wp}/R_{exp}$), and the shape parameters (u , v , w) for the studied samples.

| Sample | R_{wp} (%) | R_p (%) | R_{exp} (%) | GOF | u | v | w |
|--------|-----------------|--------------|------------------|------|----------|----------|--------|
| DG | 20.23 | 25.8 | 14.15 | 1.43 | 0.0023 | - 0.0123 | 0.0134 |
| ANN | 18.48 | 7.23 | 14.28 | 1.29 | 0.0026 | - 0.0461 | 0.1451 |
| SPS | 23.36 | 13.42 | 19.53 | 1.19 | - 0.0375 | - 0.0369 | 0.1639 |

References:

[1] Lutterotti, L.; Scardi, P. Simultaneous structure and size-strain refinement by the Rietveld method. *J. Appl. Crystallogr.* 23, (1990) 246–252.