

Supplementary Materials

Impact of Zn addition on structural, morphological, and magnetic properties of thermally annealed Li–Zn nanoferrite

S. N. Kane^a, R. Verma^a, C. Parmar^a, S. S. Modak^a, J. P. Araujo^b, F. Mazaleyrat^c, Tetiana Tatarchuk^{d,c*}

^a*Magnetic Materials Laboratory, School of Physics, D. A. University, Khandwa Road Campus, Indore-452001, India*

^b*IFIMUP, Departamento de Fisica, Universidade de Porto, 4169-007 Porto, Portugal*

^c*SATIE, ENS Paris-Saclay, Gif-sur-Yvette, France*

^d*Faculty of Chemistry, Jagiellonian University, 30-387 Kraków, Poland*

^e*Educational and Scientific Center of Materials Science and Nanotechnology, Vasyl Stefanyk Precarpathian National University, 76018 Ivano-Frankivsk, Ukraine*

CONTACT S. N. Kane, kane_sn@yahoo.com, Magnetic Materials Laboratory, School of Physics, D. A. University, Khandwa Road Campus, Indore-452001, India

Tetiana Tatarchuk, tatarchuk.tetyana@gmail.com, Faculty of Chemistry, Gronostajova str., 2, Jagiellonian University, 30-387 Kraków, Poland; Educational and Scientific Center of Materials Science and Nanotechnology, Vasyl Stefanyk Precarpathian National University, Shevchenko str., 52, 76018 Ivano-Frankivsk, Ukraine

Lattice parameter (a_{exp}) corresponding to [311] reflection was obtained by:

$$a_{\text{exp}} = d\sqrt{h^2 + k^2 + l^2} \quad (1)$$

where d – inter-planar spacing, (h, k, l) – Miller indices.

X-ray density (ρ_{XRD}) was calculated by:

$$\rho_{\text{XRD}} = \left(\frac{8M_w}{Na^3} \right) \quad (2)$$

where M_w – molecular weight, NA – Avagrado's number, a – lattice parameter.

Specific surface area 'S' was obtained by the following expression:

$$S = \frac{6}{\rho_{\text{XRD}} \times D_{\text{W-H}}} \quad (3)$$

where ρ_{XRD} – X-ray density, $D_{\text{W-H}}$ – Grain diameter.

Dislocation density was computed by the following expression:

$$\rho_{\text{D}} = 15\varepsilon / (a_{\text{exp.}} \times D_{\text{W-H}}) \quad (4)$$

Grain diameter ($D_{\text{W-H}}$) was obtained by the Williamson–Hall (W-H) method, by incorporating both instrumental and strain broadening. Instrumental broadening was calculated by taking the XRD data of the standard LaB_6 Sample. According to this method, x-ray diffraction peak broadening $\beta_{\text{hkl}} = \beta_{\text{size}} + \beta_{\text{strain}}$. The actual peak broadening (β) is obtained by correcting the experimental peak broadening ' β_{ex} ' and the instrumental broadening ' β_{in} ' as: $\beta^2 = \beta_{\text{ex}}^2 - \beta_{\text{in}}^2$. Hence, XRD peak broadening $\beta_{\text{hkl}} = \beta_{\text{size}} + \beta_{\text{strain}}$ equation (13) can be in modified form as:

$$\beta_{\text{hkl}} = (0.94\lambda / D_{\text{W-H}} \cos\theta) + 4\varepsilon \tan\theta \quad (5)$$

and

$$\beta_{\text{hkl}\cos\theta} = (0.94\lambda / D_{\text{W-H}}) + 4\varepsilon \sin\theta \quad (6)$$

where λ – wavelength of x-ray used, β – full width at half maximum ' $FWHM$ ', $D_{\text{W-H}}$ – Williamson Hall grain diameter, ε – strain.

Obtained cationic distribution was used to compute Néel magnetic moment ' \mathbf{nN} ', theoretical magnetization at 0 K: $M_{\text{s(th)}}$, is calculated by using the formula: $nN = M_{\text{B}} - M_{\text{A}}$ in Bohr magneton ' μ_{B} ' where M_{A} , M_{B} are respectively magnetic moments of A, B-site obtained

by cationic distribution. Conversion of $M_{s(th)}$ from μ_B to Am^2/kg is done using the following expression: $M_{s(th)} = [q \times \mu_B \times N_A] / m$, where, q - Neel magnetic moment, $\mu_B - 0.9274 \times 10^{-20}$ emu, N_A - Avogadro's number, m - molecular weight ($g \text{ mol}^{-1}$).

The interionic distances between cations – b, c, d, e, f , and between cation and anion – p, q, r, s were estimated the a_{exp} and $u^{\bar{4}3m}$ by using the following relations:

$$\begin{aligned} b &= \frac{a_{exp} \cdot \sqrt{2}}{4}, & p &= a_{exp} \cdot \left(\frac{5}{8} - u^{\bar{4}3m} \right) \\ c &= \frac{a_{exp} \cdot \sqrt{11}}{8}, & q &= a_{exp} \cdot \sqrt{3} \cdot \left(u^{\bar{4}3m} - \frac{1}{4} \right) \\ d &= \frac{a_{exp} \cdot \sqrt{3}}{4}, & r &= a_{exp} \cdot \sqrt{11} \cdot \left(1 + u^{\bar{4}3m} \right) \\ e &= \frac{3a_{exp} \cdot \sqrt{3}}{8}, & s &= a_{exp} \cdot \sqrt{3} \cdot \left(\frac{u^{\bar{4}3m}}{3} + \frac{1}{8} \right) \\ f &= \frac{a_{exp} \cdot \sqrt{6}}{4} \end{aligned} \quad (7)$$

where, a_{exp} – experimental lattice parameter, and $u^{\bar{4}3m}$ – oxygen position parameter.

Theoretical lattice parameter a_{th} , bond angles – $\theta_1, \theta_2, \theta_3, \theta_4, \theta_5$, oxygen position parameter – $u^{\bar{4}3m}$ were also computed by cationic distribution, utilizing the following equations:

$$a_{th} = \frac{8}{3\sqrt{3}} [(r_A + R_0) + \sqrt{3}(r_B + R_0)] \quad (9)$$

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

$$u^{\bar{4}3m} = \frac{(r_A + R_0)}{(\sqrt{3} \cdot a_{exp})} + \frac{1}{4} \quad (10)$$

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

$$\left. \begin{aligned} \theta_1 &= \cos^{-1} \left[\frac{p^2 + q^2 - c^2}{2pq} \right], & \theta_2 &= \cos^{-1} \left[\frac{p^2 + r^2 - e^2}{2pr} \right], & \theta_3 &= \cos^{-1} \left[\frac{2p^2 - b^2}{2p^2} \right] \\ \theta_4 &= \cos^{-1} \left[\frac{p^2 + s^2 - f^2}{2ps} \right], & \theta_5 &= \cos^{-1} \left[\frac{r^2 + q^2 - d^2}{2rq} \right] \end{aligned} \right\} \quad (11)$$

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

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

$$\alpha_{Y-K} = \text{Cos}^{-1} \{ (n_{B(x)}^e + M_{A(x)}) / M_{B(x)} \} \quad (12)$$

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

Anisotropy constant K_1 was calculated by using the equation:

$$K_1 = [H_c \times M_s] / 0.96 \quad (13)$$

Where M_s – Saturation magnetization, H_c - coercivity

Switching field distribution SFD is determined by using the expression:

$$SFD = \Delta H / H_c, \quad (14)$$

Where, ΔH – full width at half maximum of the dM / dH .