93522206 g

96885360 h

Supplementary Information for

Structural, optical, elastic and electrical study of spinel $Li_{0.5}ZnFe_{1.5}O4$ nanoparticles, annealed at two distinct temperatures.

D. Bouokkeze[a], J. Massoudi[b], W. Hzez[a], M. Smari[b], K. Khirouni[a], E. Dhahri[b] and L. Bessais[c].

[a] Laboratoire de Physique des Matériaux et des Nanomatériaux appliquée à l'Environnement, Faculté des Sciences de Gabès cité Erriadh, Université de Gabès, 6079 Gabès, Tunisia

[b]Laboratoire de Physique Appliquée, Faculté des Sciences de Sfax, Université de Sfax, B.P. 1171, Sfax 3000, Tunisia

[c]ICMPE (UMR 7182), CNRS, UPEC, Université Paris Est, 94320 Thiais, France

Structural properties:

- The bulk density of the annealed samples was calculated according to the standard relation:[1]

$$\rho_{th} = \frac{m}{\pi . r^2 . t} \qquad \text{S1}$$

where t and r are the thickness and radii of the prepared pellets

- The X-ray density ($\rho_{X\text{-}ray}$) of the $Li_{0.5}ZnFe_{1.5}O_4$ ferrite at different annealing temperatures was calculated as follows:[2]

$$\rho_{X-ray} = \frac{8.M}{N_A.a^3} \qquad \text{S2}$$

where M is the molecular weight of the studied ferrites, N_A is the Avogadro's number and a is the cell parameter.

- The porosity has been calculated using following standard relation:[2]

$$P(\%) = \frac{\rho_{X-ray} - \rho_{th}}{\rho_{X-ray}} \times 100 \qquad \text{S3}$$

- The specific surface area has been calculated from the following relation:[3]

$$S = \frac{6000}{D_{SC}.\rho_{X-ray}} \qquad \text{S4}$$

where D_{SC} is the diameter of the particle in nm and $\rho_{X\text{-ray}}$ is the density of the particle in g/cm^3.

- For cubic spinel structures, the hopping length between the magnetic ions in the tetrahedral (A) site (L_A) and in the octahedral [B] site (L_B), the tetrahedral (A) site radii (r_A), octahedral (B) site radii (r_B), tetrahedral and octahedral bond lengths (d_{AX} and d_{BX}), tetrahedral edge, shared and unshared octahedral edge (d_{AXE}, d_{BXE}, d_{BXEU}) were evaluated using the values of true lattice parameter 'a_0', oxygen positional parameter 'u' (u = 0.381Å), oxygen ion radius R_O(1.32Å) are obtained by the following relations:[2]

$$r_A = a\sqrt{3}(u - 0.25) - R_O \qquad \text{S5}$$

$$r_B = a(0.625 - u) - R_O \qquad \text{S6}$$

$$R_A = a\sqrt{3}(u - 0.25) \qquad \text{S7}$$

$$R_B = a(0.625 - u) \qquad \text{S8}$$

$$d_{AE} = a\sqrt{2}\left(2u - \frac{1}{2}\right) \qquad \text{S9}$$

$$d_{AL} = a\sqrt{3}\left(u - \frac{1}{4}\right) \qquad \text{S10}$$

$$d_{BL} = a\sqrt{3(u\ )^2 - \frac{11}{4}u + \frac{43}{64}} \qquad \text{S11}$$

$$d_{BE} = a\sqrt{2}(1-2u) \qquad \text{S12}$$

$$d_{BEu} = a\sqrt{4(u)^2 - 3u + \frac{11}{16}} \qquad \text{S13}$$

$$L_A = \frac{a\sqrt{3}}{4} \qquad \text{S14}$$

$$L_B = \frac{a\sqrt{2}}{4} \qquad \text{S15}$$

Elastic properties:

- The elastic modulus has been corrected using Hasselman and Fulrath model:[4]

$$1/E_0 = 1/E\left(1 - \frac{3f(1-\sigma)(9+5\sigma)}{2(7-5\sigma)}\right)$$

$$1/G_0 = 1/G\left(1 - \frac{15f(1-\sigma)}{(7-5\sigma)}\right)$$

$$\sigma_0 = \frac{E_0}{2G_0} - 1$$

$$B_0 = \frac{E_0 G_0}{3(3G_0 - E_0)}$$

- The elastic modulus has been corrected using Ledbetter and Datta model:[4]

$$G_0 = \left(\frac{1}{2A_1}\right)\left(-A_2 + \left(A_2^2 - 4A_1A_3\right)^{1/2}\right)$$

$$B_0 = \frac{4G_0B}{(4(1-f)G_0 - 3fB)}$$

$$E_0 = \frac{9B_0G_0}{G_0 + 3B_0}$$

where,

$$A_1 = \frac{8}{3}(1-f)$$

$$A_2 = (3-2f)B - (8/3+4f)G$$

$$A_3 = -3(1+f)BG$$

- Based on elastic theory and at a lower range of porosity, the linear relation between elastic moduli as a function of porosity can be written as:[4]

$$V_l = V_{l0}(1-C_l f)$$

$$V_t = V_{t0}(1-C_S f)$$

$$E = E_0(1-C_E f)$$

$$G = G_0(1-C_G f)$$

$$\sigma = \sigma_0(1-C_\sigma f)$$

where C_l, C_s, C_E, C_G and C_σ are constants of the material. The subscript '0' denotes the non-porous elastic constant of the material. Exact expressions for the constants are as follows:

$$C_l = \frac{1}{2}\left[\left|\frac{\{C_E + 2C_\sigma \sigma_0{}^2(2-\sigma_0)\}}{(1-\sigma_0)(1+\sigma_0)(1-2\sigma_0)} - 1\right|\right]$$

$$C_S = \frac{1}{3}$$

$$C_E = \left(\frac{1}{18}\right).(29+11\sigma_0)$$

$$C_G = \frac{5}{3}$$

$$C_\sigma = \left(\frac{5}{9}\right) + \left(\frac{11\sigma}{18}\right) - \left(\frac{1}{18}\sigma\right)$$

.

The above relations are used to determine the elastic moduli for non-porous material, and the results are shown in table S1.

Table S1: The elastic moduli for non-porous material of Li-Zn ferrite annealed at 500 and 1100 °C.

Model	Parameter	Zn500	Zn1100
Hasselman and Fulrath model	E_0 (GPa)	471	411
	G_0 (GPa)	164	147
	σ_0	0.43	0.40
	B_0 (GPa)	1189	699
Ledbetter and Datta model	E_0 (GPa)	402	379
	G_0 (GPa)	144	137
	B_0 (GPa)	655	551
	A_1	2.04	2.19
	A_2	367	446
	A_3	-94777	-101981
Elastic theory	E_0 (GPa)	446	396
	G_0 (GPa)	152	139
	V_{l0} (m/s)	10925	10245
	V_{t0} (m/s)	4725	4784
	V_{m0} (m/s)	5338	5386
	σ_0	0.42	0.40
	C_l	1.31	1.34
	C_E	1.867	1.855
	C_σ	0.75	0.75

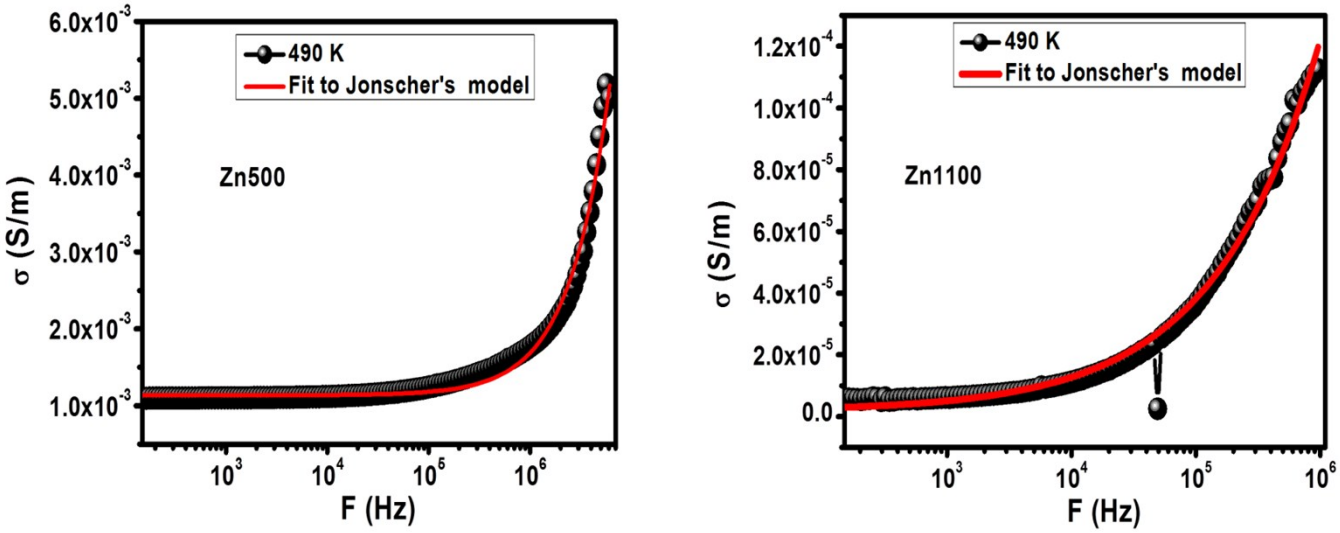

Fig. S1 Conductivity spectra at 490k of Zn500 and Zn1100.

Reference:

1M.J. Iqbal, S. Farooq, Mater. Sci. Eng. B., 2007, 136, 140.
2 V.K. Lakhani, T.K. Pathak, N.H. Vasoya, K.B. Modi, Solid State Sciences., 2011, 13, 539-547
3M. Georgea, A.M.Johna, S. S. Naira, P.A. Joyb, M.R. Anantharaman, Journal of Magnetism and Magnetic Materials.,2006, 302, 190-195
4 P. U. Sharma and K. B. Modi, Phys. Scr., 2010, 81, 015601