Electronic supplementary information

Cation distribution a key to ascertain the magnetic interactions in cobalt substituted Mg-Mn nanoferrite matrix

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The X-ray intensity for different planes (I_{hkl}) for powder specimen was calculated by using following relation:

$$I_{hkl} = |F|^2_{hkl}.P.L_p \quad \text{(S1)}$$

where F is structure factor, P is multiplicity factor and L_p is Lorentz polarization factor. The Lorentz polarization factor was calculated by using the following relation:

$$L_p = \left(\frac{1+cos^2 2\theta}{sin^2\theta\, cos\theta}\right) \quad \text{(S2)}$$

$$\left(Mg_{0.9-x}Mn_{0.1-y}Co_{z-\delta}Fe_{1-\delta}\right)_A\left[Mg_xMn_yCo_\delta Fe_{1-z+\delta}\right]_B O_4 \quad \text{(S3)}$$

$$r_A = \left[C_{AMg}r(Mg^{2+}) + C_{AMn}r(Mn^{2+}) + C_{AFe}r(Fe^{3+}) + C_{ACo}r(Co^{2+})\right] \quad \text{(S4)}$$

$$r_B = \frac{\left[C_{BMg}r(Mg^{2+}) + C_{BMn}r(Mn^{2+}) + C_{BFe}r(Fe^{3+}) + C_{BCo}r(Co^{2+})\right]}{2} \quad \text{(S5)}$$

$$a_{th} = (8/3\sqrt{3})\,[(r_A + R_o) + \sqrt{3}\,(r_B + R_o)] \quad \text{(S6)}$$

$$T = \frac{1}{\sqrt{3}}\left(\frac{r_A + R_o}{r_B + R_o}\right) + \frac{1}{\sqrt{2}}\left(\frac{R_o}{r_A + R_o}\right) \quad \text{(S7)}$$

$$u^{3m} = \frac{\frac{1}{4}R^2 - \frac{2}{3} + \sqrt{\left(\frac{11}{48}R^2 - \frac{1}{18}\right)}}{2R^2 - 2} \quad \text{(S8)}$$

$$u^{\bar{4}3m} = \frac{\frac{1}{2}R^2 - \frac{11}{12} + \sqrt{\left(\frac{11}{48}R^2 - \frac{1}{18}\right)}}{2R^2 - 2} \quad \text{(S9)}$$

$$u^{\bar{4}3m} = \left[\frac{1}{a_{th}\sqrt{3}}(r_A + R_o) + \frac{1}{4}\right] \quad \text{(S10)}$$

where $R = \frac{(B-O)}{(A-O)}$.

The bond lengths *B*-*O* and *A*-*O* are average bond lengths calculated based on the cation distribution; where $B - O = \langle r_B + R_o \rangle$ and $A - O = \langle r_A + R_o \rangle$.

$$d_{AX} = a\sqrt{3}\left(U - \frac{1}{4}\right) \quad \text{(S11)}$$

$$d_{BX} = a\left[3U^2 - \left(\frac{11}{4}\right)U + \frac{43}{64}\right]^{1/2} \quad \text{(S12)}$$

$$d_{AXE} = a\sqrt{2}\left(2U - \frac{1}{2}\right) \quad \text{(S13)}$$

$$d_{BXE} = a\sqrt{2}(1 - 2U) \quad \text{(S14)}$$

$$d_{BXEU} = a\left(4U^2 - 3U + \frac{11}{16}\right) \quad \text{(S15)}$$