CATION DISTRIBUTION IN CUFE2O4 AND ZNFE2O4 FINE PARTICLES STUDIED BY RIETVELD STRUCTURE REFINEMENT OF THE SYNCHROTRON X-RAY POWDER DIFFRACTION

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Magnetic properties of nanosized ferrite particles are a subject of great interest due in part to their use in high-density storage but also in biological applications. Spinel ferrites have the general molecular formula \( (M^{2+}) \{Fe^{3+}\}^2 \{O^2-\}^4 \) where \( M^{2+} \) and \( Fe^{3+} \) are the divalent and trivalent cations occupying tetrahedral (A) and octahedral (B) interstitial positions of the fcc lattice formed by \( O^2- \) ions. Nevertheless, a whole range of cations distribution is possible in spinels and they are better represented by the more precise formula \( (M^{2+})^{x} \{Fe^{3+}\}^{1-x} \{M^{2+}\}^{x} \{Fe^{3+}\}^{2-x} \{O^2-\}^4 \), where the ions inside the brackets are said to occupy B-sites and the ions outside the bracket occupy A-sites. Then, \( x \) represents the so-called degree of inversion also defined as the fraction of A-sites occupied by \( Fe^{3+} \) cations. Changes in cation distribution in this type of compounds confer special characteristics and properties, particularly, in magnetic properties. In this work, nanocrystalline CuFe\(_2\)O\(_4\) and ZnFe\(_2\)O\(_4\) spinels have been chemically synthesized with various grain sizes, using hydrothermal coprecipitating aqueous solutions of \( Fe^{3+} \) and \( M^{2+} \) (\( M^{2+} = Cu^{2+} \) and \( Zn^{2+} \)) mixture in alkaline medium, in order to elaborate magnetic fluids. Rietveld structure refinement of x-ray powder diffraction data is used to determine the cation distribution of our nanostructures. Our results show that zinc occupies B-sites with a value of \( x \) around 0.22, in good agreement with magnetization data [1]. Copper ferrite nanoparticles are found to have a mixed spinel structure and the result is compared with those obtained by Mössbauer spectroscopy measurements in the presence of an applied magnetic field. Moreover, the quality of these last results is improved using the Rietveld structure refinement of synchrotron x-ray powder diffraction data. [1] J.A. Gomes, M.H. Sousa, F.A. Tourinho, J. Mestnik-Filho, R. Itri and J. Depeyrot. J. Metastable Nanocrystalline Materials, In Press (2003).