Antistructure Modelling of $CoFe_2O_4$ Nanoparticles Prepared by Precipitate Method

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Spinel ferrite are intensively studied for their good magnetic property and stable chemical property. They shows typical ferromagnetic property at room temperature and it is wildly use as magnetic carrier in adsorbent to realize magnetic separation. Applications of ferrites of nanometer size have prompted the development of several widely used methods, including sol-gel techniques, reverse micelles, co-precipitation, citrate precursor techniques and other, for the fabrication of spinel ferrite nanoparticles.

In this work, the nanocrystalline $CoFe_2O_4$ was prepared using chemical co-precipitation method. The starting materials $Fe(NO_3)_2 \cdot 9H_2O$ and $Co(NO_3)_2 \cdot 6H_2O$ were dissolved in 700 ml of distilled water by intensive stirring, accordingly a homogeneous solution was obtained, and then NaOH was added to the solution until the pH 11,5. After the completion of the reaction, the solid product washed several times with deionized water. The final product was dried oven at 100 °C for 6 h, then was calcined at 800 ◦C for 2 h. Black powders were obtained and characterized as nanocrystalline $CoFe_2O_4$ ferrites.

The powder X-ray diffraction (XRD) patterns were recorded by use of a DRON-3 diffractometer with $Cu_{K\alpha}$ radiation (λ = 1,5406 Å). The diffraction patterns of the sample shows the formation of the spinel phase with cubic structure. In order to calculate the crystallite size, the Scherrer's method was applied. The thermal behavior of powder precursor was characterized by Differential Scanning Calorimetry (DSC) and Thermo-Gravimetric Analysis (TGA) in order to analyze the mass loss and possible energy transitions. The endothermic peak in the DSC curve can be explained by the loss of water (OH-groups), the exothermic peak corresponds to the crystallization of the spinel. The morphologies of obtained sample have been characterized by scanning electron microscopy.

According to crystalloquasichemical model [1], the nature of defects and the mechanism of interaction between CoO and Fe_2O_3 oxide phases during the formation of cobalt ferrite spinel structure was described. Processes on the surface CoO and Fe_2O_3 are treated separately with the formation of CoO and Fe_2O_3 defective phases respectively:

$$(1-\alpha)Co_{Co}^{\times}O_O^{\times} + \alpha\left(Fe_{2/3}^{\bullet}V_{1/3}''\right)_{Co}O_O^{\times} \rightarrow \left(Co_{1-\alpha}^{\times}Fe_{2/3\alpha}^{\bullet}V_{1/3\alpha}''\right)_{Co}O_O^{\times} \quad ,$$

$$(1-\gamma)\left(Fe_2^{\times}\right)_{Fe}\left(O_3^{\times}\right)_O + \gamma\left(Co_2'\right)_{Fe}\left(O_2^{\times}V^{\bullet\bullet}\right)_O \rightarrow \left(Fe_{2-2\gamma}^{\times}Co_{2\gamma}'\right)_{Fe}\left(O_{3-\gamma}^{\times}V_{\gamma}^{\bullet\bullet}\right)_O \quad ,$$

where $\bullet$ is an excess positive charge, $'$ and $''$ is a single and double excess negative charge respectively, V_{Co}'' – cation vacancy, $V_O^{\bullet\bullet}$ – anion vacancy, $\times$ is an effective zero charge.