

Nanocomposites and nanomaterials

Estimating the Cation Distributions in $\text{Co}_x\text{Zn}_{1-x}\text{Fe}_2\text{O}_4$ Ferrites Using X-Ray, FT-IR and Mössbauer spectroscopy

T.R. Tatarchuk¹, N.D. Paliychuk¹, I.P. Yaremiy²

¹ Department of Inorganic and Physical Chemistry, Institute of Natural Science, Vasyl Stefanyk Precarpathian National University, Shevchenko Str., 57, Ivano-Frankivsk-76018, Ukraine.

E-mail: tatarchuk.tetyana@gmail.com

² Physical and Technical Department, Vasyl Stefanyk Precarpathian National University, Shevchenko Str., 57, Ivano-Frankivsk-76018, Ukraine.

Nanoparticles of spinel ferrites are in particular interesting for both fundamental and applied science. The properties of Co–Zn ferrite depend mainly on the technique and conditions of preparation, which in turn affect the cation distribution over the tetrahedral A–site and the octahedral B–site. In this work the cation distribution of $\text{Co}_x\text{Zn}_{1-x}\text{Fe}_2\text{O}_4$ were studied using the X-ray diffraction, FT-IR and Mössbauer spectroscopy.

The lattice constant “a” decreases from 0,843 nm for ZnFe_2O_4 to 0,835 nm for CoFe_2O_4 spinels. Using the experimental values of lattice parameter a , oxygen positional parameter u , tetrahedral and octahedral bond lengths, tetrahedral edge, shared and unshared octahedral edges were calculated. The FT-IR results show the presence of two vibrational modes in the frequency range of 400–4000 cm^{-1} corresponding to tetrahedral and octahedral sites. The scanning electron microscope (SEM) micrographs showed aggregates of stacked large grains. The average crystallite size of the nanoparticles was calculated with use of the Scherrer equation and the Williamson–Hall method. The presence of paramagnetic doublet in the ^{57}Fe Mössbauer spectra may be attributed to the small particle size. It is seen that the isomer shift values of the A site are less than those of the B site.

The crystalloquasichemical mechanism of formation stoichiometric cobalt ferrite through interaction by defective hydroxide phases was described. Crystalloquasichemical modeling of surface interactions between $\text{Co}(\text{OH})_2$ and $\text{Fe}(\text{OH})_3$ can trace the formation of spinel structure with the participation of antistructure of matrix and reduced to the corresponding stoichiometric hydroxides species, for example: