Coercivity dependence of cation distribution in Co-based spinel: Correlating theory and experiments

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Abstract
The inversion degree (X) of a spinel-type nanomaterial is an essential parameter to understand the magnetic and electronic properties of ferrites. In this work, we have related different theoretical and experimental approaches in order to know the X parameter of a Co-based spinel. Our hypothesis is that the hysteresis curve at 5 K may be used to find the X parameter taking into consideration that the coercivity and remanence of this kind of nanoparticle (NP) are strongly dependent on the cation distribution between A and B sites of the spinel structure. To investigate this, CoFe2O4 NPs were firstly synthesized and fully characterized by powder X-ray diffraction (PXRD), transmission electron microscopy (TEM), and vibrating sample magnetometry (VSM). These results pointed out monodisperse CoFe2O4 nanostructures with a spherical shape of 6.85 ± 0.05 nm. Subsequently, first-principles calculations were carried out to obtain the most stable atomic configuration as a function of the level of inversion, as well as the atomic properties for each X. Then, these data were used to define the constants used in the micromagnetic calculations. A hysteresis loop was generated for each X and further compared to the experimental curve measured at 5 K. In this sense, the best fit was found for X = 0.75, which indicates this value as the most probable inversion degree for the CoFe2O4 nanostructures investigated in this work. Overall, we are able to connect the experiments with the atomistic explanation through micromagnetic simulations in order to find the cationic configuration of the Co-based spinel nanostructure.

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