

Investigation of Hyperfine Interactions of Multiferroic Oxides Bi_{0.85}La_{0.15}FeO₃ Through Perturbed Angular Correlation Spectroscopy

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1. Introduction

Multiferroic materials exhibit ferroelasticity (stress-strain hysteresis ratio) along with magnetic ordering and ferroelectricity, with magnetic-electrical coupling, which have attracted enormous curiosity because of their possible applications in magnetoelectric devices and next-generation memory storage media [1]. The bismuth ferrite BiFeO₃ is a known multiferroic compound because of its potential for practical, antiferromagnetic and ferroelectric application with ordering temperatures above ambient temperature (ferroelectric Curie temperature, $T_C \sim 830$ °C and antiferromagnetic Néel temperature $T_N \sim 370$ °C) [2].

In this work, powder samples $Bi_{0.85}La_{0.15}FeO_3$ (BLFO15) were synthesized by the sol-gel method, in order to investigate, within an atomic scale, the ferromagnetic and electrical dependencies on temperature by using measuring hyperfine interactions, through techniques such as Perturbed γ - γ Angular Correlation (PAC) [3], as well as Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD) and Rietveld refinement.

2. Methodology

Hyperfine interactions are at the origin of the spectral hyperfine structure that can be observed with various techniques. The term hyperfine structure refers to small changes and divisions in atomic, ionic, or molecular energy levels that result from the nucleus' interactions with electrical and magnetic fields external to the nucleus [4].

These effects were first observed in optical spectra and turned out to be much smaller than those considered as the fine structure, which arises from the interaction between the magnetic moments associated with the electron spin and the orbital angular momentum of the electron. Since the hyperfine division energy is much less than the spin-orbit coupling energy, the associated transition frequencies are generally not in the optical frequency range, but in the microwave or radio frequency range. In order of importance, the magnetic dipole and electrical quadrupolar interactions are dominant and, therefore, the most studied of the hyperfine interaction. The hyperfine interaction Hamiltonian (H_{HF}) can be written as the sum of two components, a magnetic (H_M) and an electrical (H_E) component:

$$H_{HF} = H_M + H_E \tag{1}$$

The electrical component appears for cases of compounds with symmetry different from the cubic, and this interaction can provide information about the local symmetry of the site where the probe is located and about the density of charges around it [5].

The disturbed gamma-gamma angular correlation spectroscopy (PAC) technique is a nuclear technique that in general investigates the hyperfine interactions of materials through radiation ($\alpha, \beta e \gamma$) emitted by an unstable radioactive nucleus, thus providing data of the hyperfine parameters of each material studied, such as: magnetic frequency (ν_M), electric quadrupole frequency (ν_Q), delta (δ), asymmetry parameter (η) and the hyperfine magnetic field (B_{HF}). These interactions occur at atomic levels where the radioactive nucleus, more commonly called the probe nucleus, causes a diffusion of energy levels from the nucleus to its lower levels (sublevels).

The technique is based on the study of magnetic and electrical hyperfine interactions between the nuclear moments of the probe core and magnetic or electric fields external to the probe core. These interactions trigger an unfolding of core energy levels into its sub-levels. The detection of transitions between these energy sublevels by means of emitted gamma radiation provides information about the electric and magnetic fields generated in the vicinity of the probe core. Experimentally, the PAC technique measures the temporal dependence of the gamma-ray emission pattern. This dependence can be created by a rotation or precession of the angular distribution of gamma radiation, and the origin of this precession is the hyperfine interaction.

3. Results and Discussion

The XRD analysis shown to the verification of the formation of the crystallines phases correspondents to Fe_2O_3 and Bi_2O_3 samples (see Fig. 1).



Figure 1: The XRD pattern of the sample $Bi_{0.85}La_{0.15}FeO_3$, between parentheses are represented the theoretical peaks of the predominant phase of Fe_2O_3 .

The SEM images show that the formation of the spurious phase of Fe_2O_3 actually occurred when compared to the literature¹ (see Fig. 2).

¹ CBQ. Disponível em <<u>http://www.abq.org.br/cbq/2012/trabalhos/12/874-14030.html</u>>. Acesso em 30 de agosto de 2021.



Figure 2: The SEM images to BLFO15 (a) and Fe_2O_3 (b).

The PAC measurement at a temperature of 400 °C shows the characteristic frequency of materials with an orthorhombic phase with only site (in red) corresponding to the Fe_2O_3 phase present in the BLFO15 sample (see Fig. 3).



Figure 3: Transformed of Fourier (F (ω)) and spectra R (t) generated thought the software TDPAC exibits the sample BLFO15 in 400 °C.

4. Conclusions

It is concluded that the formation of the desired phase of $BiFeO_3$ in doping with 15% of La did not occur. Checking the XRD for the formation of a phase of Fe_2O_3 (predominant) and Bi_2O_3 (probably on the surface of the sample). The SEM analysis confirmed the formation of the Fe_2O_3 phase as well as the PAC analysis, being necessary a more in-depth study than occurred during the synthesis. One hypothesis was the use of 5 drops of hydrochloric acid in the nitric acid and metallic Fe solution, which possibly favored the formation of impurities.

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