Experimental report

21/12/2023

Proposal: **5-31-2682** **Council:** 4/2019

Title: Structural and magnetic characterization in 6H-BaFeO3

Research area: Materials

This proposal is a new proposal

Main proposer: **Maria HERNANDO GONZALEZ**

Experimental team: Maria HERNANDO GONZALEZ
Daniel GUTIERREZ

Local contacts: Maria Teresa FERNANDEZ DIAZ

Samples: BaFeO3

Instrument	Requested days	Allocated days	From	To
D2B	1	1	10/09/2019	11/09/2019
D20	1	1	16/09/2019	17/09/2019

Abstract:

The 6H-BaFeO3-x system is known by their structural complexity. In fact, little variations on the oxygen content leads to slight but significant structural modification of the 6H-type structure. For that, we consider very interesting to study a sample with all Fe in the IV oxidation state. In this sense, we have prepared 6H-BaFeO3 (x=0). The magnetic measurements show a complex and rich magnetic behavior for 6H-BaFeO3 sample and a disproportionation of FeIV in FeIII and FeV. Taking into account that the synthesized BaFeO3 material is the most oxidized sample up to now reported, the aim of this work is to get more information about their structural and magnetic behavior at room and low temperatures. These results allow us to stablish the structural effects originated by the Fe(IV) disproportionation at low temperature. For this proposal, to follow the thermal evolution of the structural and magnetic phase we need collect diffraction data at D20 high flux powder diffractometer and in D2B at 2, 130, 215 and 300 K.

It is well known that 6H-type BaFeO3-x has attracted much attention because its electronic and magnetic states are very complicated [1-3].The 6H-BaFeO3-x system is known by their structural complexity. In fact, little variations on the oxygen content leads to slight but significant structural modification of the 6Htype structure. Up to know, the more oxidized sample reported is close to BaFeO2.9 (x~ 0.1), i.e. containing Fe4+ and Fe3+. For that, we consider very interesting to study a sample with all Fe in the IV oxidation state. In this sense, we have prepared 6H-BaFeO3 (x=0).

The NPD data collected at room temperature on D2B diffractometer were refined on the basis of P63/mmc symmetry (hexagonal) figure 1. The result of the refinement reflects that the sample adopts the ideal 6H structure with BaFeO2.96 composition.

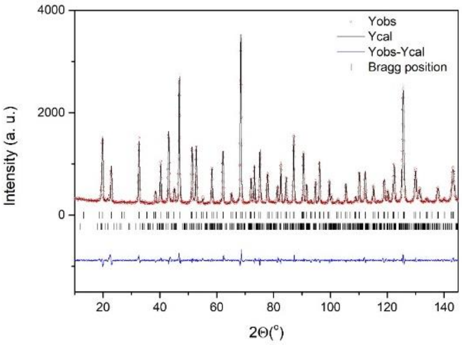

Figure 1. Rietveld refinement of the NPD data measured at RT for 6H-BaFe$O_{2.96}$ oxide. The observed (red circles) and calculated patterns (continuous black line) and difference curves (continuous blue line) are shown.

The possible structural and magnetic transitions below room temperature were investigated by neutron diffraction measurements in D20 diffractometer using two different wavelength (λ=1.54 and 2.4 Å). Data collected with λ=1.54 Å over different temperature values between 50 and 300K show that below 150 K extra peaks appear in the ND patterns that correspond to long range magnetic order, see figure 2.

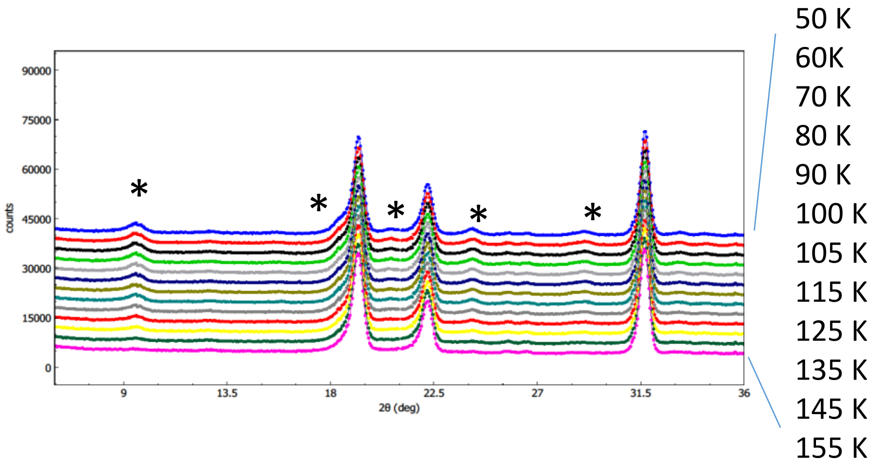

Figure 2. Neutron diffraction patterns from 155 K to 50 K of the $BaFeO_{2.96}$. The magnetic reflections are marked with an asterisk.

Different neutron diffraction data have been refined from 160 K and we are analyzing the variation of the structural parameters in order to study the possible structural changes associated to the FeIV disproportionation phenomenon previously reported from Fe Mossbauer spectroscopy results [4].

Neutron diffraction patterns recorded below 160 K contain scattering contributions to the Bragg peaks could be magnetic in origin. In order to solve the magnetic structure, neutron diffraction data were collected below 150 K with wavelength of 2.4 Å at the diffractometer D20. The data recorded at 10 K are shown in the figure 3. The resolution of the such complex magnetic structure is in progress.

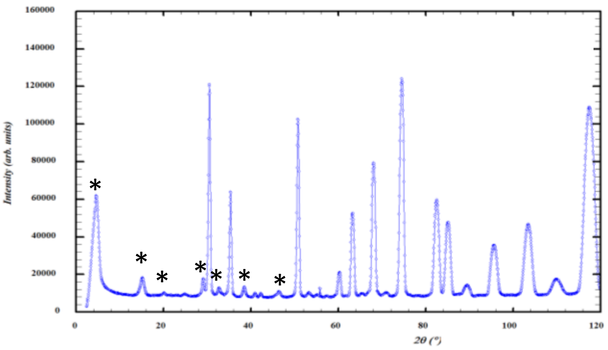

Figure 3. Neutron diffraction patterns at 10 K of the $BaFeO_{2.96.}$ The magnetic reflections are marked with an asterisk.

[1] K. Mori et al, J. Appl. Cryst. (2007) 40, s501–s505.

[2] F. lga et al, Journal of Magnetism and Magnetic Materials (1992) 104-107 1973-1975.

[3] K. Mori et al, Physica B (2003) 329–333 807–808.

[4] H. Kobayashi et al, Nuclear Instruments and methods in physics research B76 (1993) 258-259.