Experimental report

06/03/2024

Proposal: CRG-2986 **Council:** 10/2022

Title: In-situ" evolution of the crystal structure of the Sr0.9Ba0.1Co1-xMxO3-d and SrCo1-x-yFexMyO3-d (M= Ti, Ir) SOFC cathodes

Research area:

This proposal is a new proposal

Main proposer: **Vanessa Amelia CASCOS JIMENEZ**

Experimental team: Maria Teresa FERNANDEZ DIAZ
Vanessa Amelia CASCOS JIMENEZ

Local contacts: Ines PUENTE ORENCH

Samples: Sr0.9Ba0.1Co1-x-yFexMyO3-d (M=Ti, Ir)

Instrument	Requested days	Allocated days	From	To
D1B	2	1	06/06/2023	07/06/2023

Abstract:

Experimental Report

15-06-2023

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Experimental Team:
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Local Contact: Puente Orench, Ines

Samples: Sr0.9Ba0.1Co1-x-yFexMyO3-d (M=Ti, Ir)

Instrument: D1B
Req. Days: 2 **All. Days:** 1
From: 06/06/2023 **To:** 07/06/2023

Abstract:
The novel perovskites Sr0.9Ba0.1Co1-xMxO3-d and SrCo1-x-yFexMyO3-d (M= Ti, Ir) have been evaluated as superior cathodes for solid-oxide fuel cells (SOFC); tests in single fuel cells yield output powers higher than 700 mW/cm2 at 850 oC with H2 as a fuel. In this experiment we aim at unravelling the oxide-ion diffusion path of this family of MIEC (mixed ionic-electronic conductor) oxides. We plan to study the thermal evolution of the crystal structure in order to get information about the actual crystal symmetry, the thermal displacements and oxygen contents, as well as the order-disorder of the oxygen vacancies and their evolution at the actual working conditions in a SOFC cell, in air at temperatures between RT and 900 oC.

The stabilization of a 3D perovskite-like framework in the $SrCoO_{3-\delta}$ system has been a widely used strategy in order to obtain an adequate mixed ionic-electronic conductor to be used as cathode in intermediate temperature solid oxide fuel cells. For this purpose, several chemical substitutions have been performed in either the Sr (Ba, La, Sm) [1] or in the Co (Sc, Ni, etc) [2,3] positions or in both. In this work we have stabilized a perovskite phase by doping the $SrCoO_{3-\delta}$ system with Fe and Ir contents in $SrCo_{0.50}Fe_{0.40}Ir_{0.10}O_{3-\delta}$. The stabilization of a cubic *Pm-3m* structure has been obtained at RT. Fig.1 illustrates the goodness of the fit for the NPD pattern for $SrCo_{0.50}Fe_{0.40}Ir_{0.10}O_{3-\delta}$ compound at RT measured at the D1B diffractometer of the ILL (Grenoble, France).

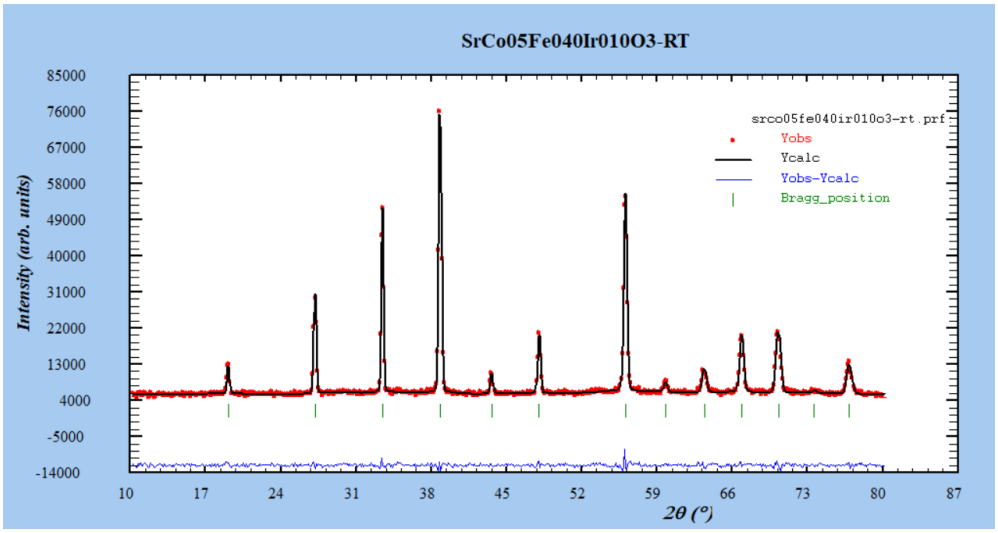

Fig. 1. *Observed (red line), calculated (black line) and difference (bottom line) NPD Rietveld profile for* $SrCo_{0.50}Fe_{0.40}Ir_{0.10}O_{3-\delta}$ *at 25 ºC.*

Besides, in this experiment we have measured the in-situ structural evolution of the samples in the usual working conditions of a cathode in a SOFC (in air from 200 ºC to 800 ºC). Neutron powder diffraction (NPD) data were collected in the diffractometer D1B. A neutron wavelength of λ= 1.2874 Å was selected within the angular 2θ range from 2° to 128°. About 1 g of the sample was contained in a quartz tube open to the ambient atmosphere, placed in the isothermal zone of a furnace with a vanadium resistor operating under vacuum. The measurements were carried out in air at 200, 300, 400, 500, 600, 700 and 800ºC. The collection time was of 3 h per pattern. The irregular background coming from the quartz container was interpolated from points devoid of reflections.

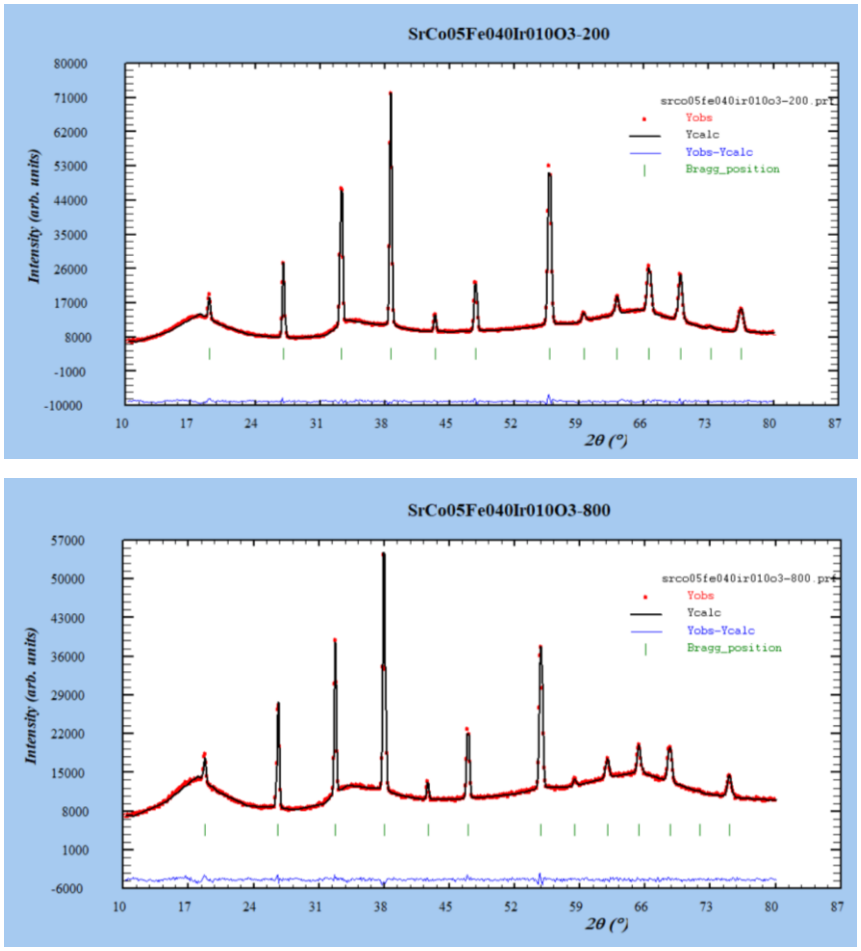

Fig. 2. *Observed (red line), calculated (black line) and difference (at the bottom) NPD profiles for* $SrCo_{0.50}Fe_{0.40}Ir_{0.10}O_{3-\delta}$ *at 200 and 800 ºC. The vertical markers correspond to the allowed Bragg reflections.*

The crystal structure is also stabilized in the cubic *Pm-3m* space group from 200 to 800 ºC (Fig. 2). No phase transition was detected in the whole range of temperatures measured.

References

[1] T. Nagai, W. Ito, TR. Sakon, Solid State Ionics 177 (2007) 3433.

[2] Z. Q. Deng, W. Liu, C. S. Chen, H. Lu, W. S. Yang, Solid State Ionics 170 (2004) 187.

[3] P. Zeng, R. Ranj, Z. Chen, W. Zhou, H. Gu, Z. Shao, S. Liu, J. Alloys and Comp., 455 (2008) 465-470.