Experimental report

26/07/2022

Proposal: **CRG-2713** **Council:** 10/2019

Title: Thermal evolution of the high-performance IT-SOFC cathode materials Nd1-xSrxCoO3-δ (x =1/3, 2/3)

Research area:

This proposal is a new proposal

Main proposer: **Ulises AMADOR**

Experimental team: Ulises AMADOR

Local contacts: Oscar Ramon FABELO ROSA

Samples: Nd1-xSrxCoO3-δ (x=1/3, 2/3)

Instrument	Requested days	Allocated days	From	To
D1B	5	2	17/02/2020	19/02/2020

Abstract:

Thermal evolution of the high-performance IT-SOFC cathode materials $Nd_{1-x}Sr_xCoO_{3-\delta}$ (x= 1/3, 2/3)

Ulises Amador and M.Teresa Azcondo

Dept. Química, Univ. San Pablo-CEU, Urb. Montepríncipe, 28668 Boadilla del Monte, Madrid, Spain.

The aim of the proposal CRG-2713 was to determine the thermal evolution in air of the two SOFC cathode materials $Nd_{1-x}Sr_xCoO_{3-\delta}$ (x= 1/3, 2/3) up to operational temperatures, in particular the oxygen content and to determine any phase transition (very likely for the x=1/3 perovskite). NPD data recorded at room temperature shown in Fig. 1 (experiment 5-24-583) showed that the x=2/3 phase presents a cubic perovskite structure with S.G. Pm-3m whereas for x=1/3 the material is orthorhombic with symmetry Pnma. Figures 1a and 1b show the corresponding NPD patterns fitted to the above commented models.

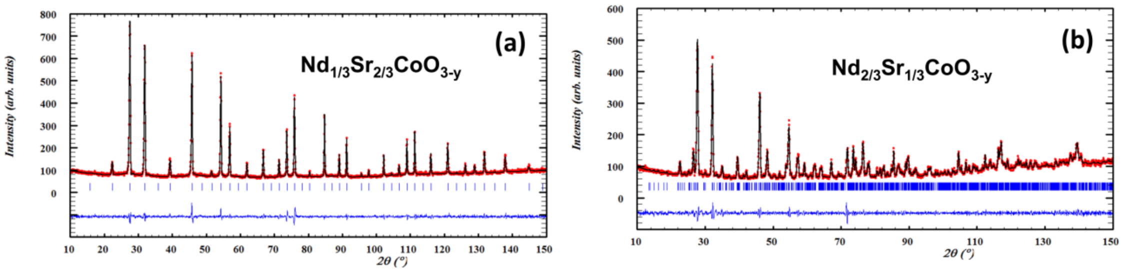

Figure 1. Experimental (red points), calculated (solid black line) and their difference (blue line at bottom) NPD diffraction patterns at RT for $Nd_{1/3}Sr_{2/3}CoO_{3-\delta}$ (a) and $Nd_{2/3}Sr_{1/3}CoO_{3-\delta}$. The vertical bars indicate the positions of the Bragg peaks.

The structural refinements allow determining the exact compositions at RT of both oxides to be: $Nd_{0.66(1)}Sr_{0.33(1)}CoO_{2.896(4)}$ and $Nd_{0.33(1)}Sr_{0.66(1)}CoO_{2.950(2)}$. The metal compositions are the nominal ones and both pristine oxides present a noticeably concentration of oxygen vacancies.

The thermodiffraction measurements conducted in the framework of the present experiment allowed to correlate the materials structures with the electrical and electrochemical properties. The results have been published in the papers: *Inorg. Chem.* **2020** *59*, 12111 (DOI: 10.1021/acs.inorgchem.0c01049). Figures 2 and 3, taken from the above paper nicely explain the superior performance of $Nd_{0.33(1)}Sr_{0.66(1)}CoO_{2.950(2)}$ since this oxide presents an optimal balance between p-charge carriers concertation (related to cobalt oxidation state) and oxygen vacancies (promoting ionic conduction).

Figure 2

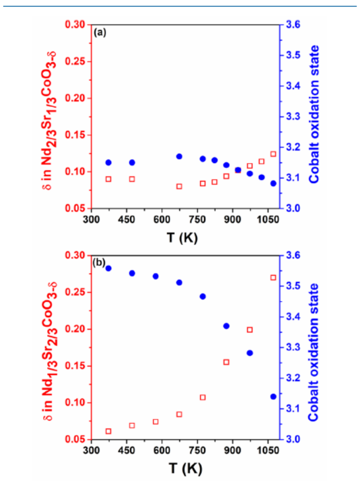

Figure 5. Thermal evolution of the oxygen content and cobalt oxidation state for (a) orthorhombic $Nd_{2/3}Sr_{1/3}O_{3-\delta}$ and (b) cubic $Nd_{1/3}Sr_{2/3}O_{3-\delta}$ in air, determined from NPD.

Figure 3

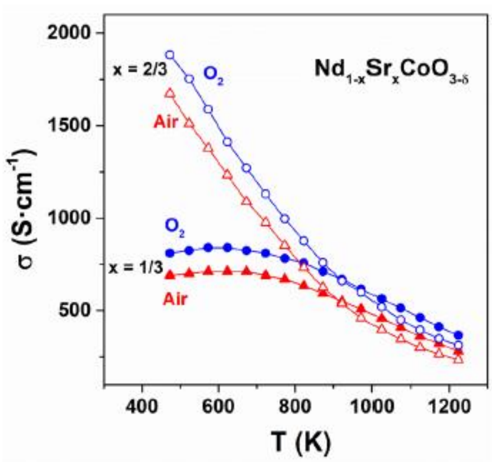

Figure 7. Electrical conductivity as a function of temperature for $Nd_{1-x}Sr_xO_{3-\delta}$ (x = 1/3, 2/3) in air and O_2.