Introduction

Solid Oxide Fuel Cells (SOFC) are a promising technology for moving towards a low carbon economy because they bring the attractive added attributes of low emissions and an inherent scalability suitable for distributed generation. Unfortunately, their working temperature is high (typically > 800 ^{o}C), resulting in materials degradation, materials selection limitations and high costs. Reducing cell operating temperature is a primary goal for the commercialization of this type of fuel cells. In this regard, recent studies have focused on operating temperatures between 550-750 °C, in order to lower the cost, by introducing metallic components as interconnectors and balance of plant, and to extend the durability of fuel cells. Unfortunately, decreasing the operating temperature gives lower cell performance due to a decrease in electrode activity and electrolyte conductivity.

The aim of this project is to gain a fundamental understanding of oxygen transport and of the basic mechanisms affecting oxygen reduction and hence the cathode performance. The knowledge acquired will be translated to other fields aiming towards **the development of alternative energy conversion and related technologies** with a direct impact in the reduction of CO_2 emissions. The new materials and the understanding of the oxygen reduction mechanisms can be directly applied to functional membranes in oxygen pumps, oxygen separation and as active interlayers and functional layers to improve the performance SOFC and electrolysers.

Results

The main results obtained are described next:

- By the use of a novel combination of electron back scattered diffraction measurements, time-of-flight, and focused ion beam SIMS, the anisotropy in the oxygen diffusion, which had been predicted by simulations, was experimentally proven for the first time.

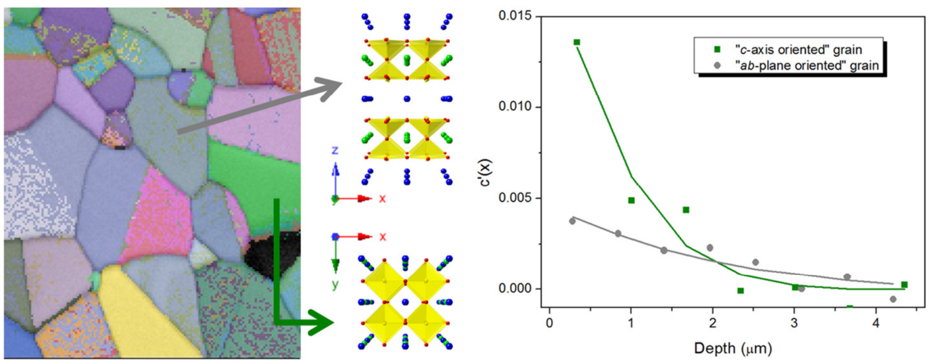

Fig. 1 (a) EBSD color-coded surface orientation image with grains A and B (measured by FIB-SIMS) marked, and b) normalized ^{18}O concentration profiles in individual grains for a PBCO pellet exchanged at 300 °C and fit to Crank's solution to Fick's second law.

- We measured oxygen diffusion coefficients for the perovskite composition LPBSFC which are higher than those for most of the cathode materials reported in the literature and they agree with the calculated ones from electrochemical impedance spectroscopy measurements. This reinforces the relevance of using the new multi-element analysis for discovering new electrode materials and the suitability of the LPBSFC material for IT-SOFC cathode and oxygen membrane applications.

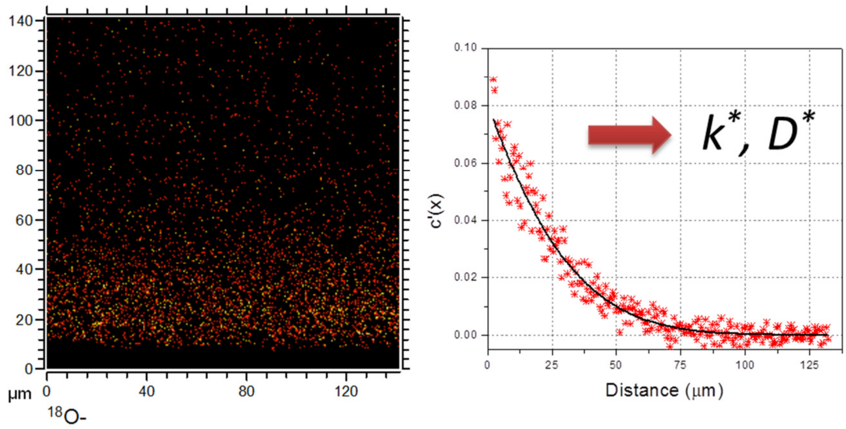

Fig 2. (a) ^{18}O surface map for the LPBSFC sample exchanged at 553 ºC; (b) normalised ^{18}O depth profile obtained from the same sample

- X-ray scattering techniques, through crystal truncation rod (CTR) experiments, have been used for the first time to probe the atomic surface structure and reconstruction/relaxation of $(La,Sr)NiO_4$ single crystals as a function of temperature. In addition, these structural models have complemented and correlated with elemental characterisation data of the outermost surface layer and with near surface depth profiles obtained by Low Energy Ion Scattering (LEIS) measurements and by XPS measurements.

- The oxygen surface exchange and diffusion properties have been measured perovskite combinatorial thin films samples. These unique results are a key part of an entire study of the variation of the cathode functional properties with composition, which proves the importance of the combinatorial approach for the optimization of the materials properties, being able to scan a wide range of materials compositions in a single thin film deposition experiment.

- The influence of cation ordering in the oxygen conduction properties has been experimentally evaluated for the first time on double perovskite epitaxial thin films.

- Pioneering work in surface science of cathode materials has been carried out. A number of cathode materials have been measured, among which we have found similar trends regarding the surface termination, surface segregation and the dependence of these with the history of the sample.

- The relationship between the surface oxygen exchange properties and the outermost surface composition and segregation for MIEC cathode materials has been simultaneously measured and evaluated for the first time. These in-depth studies have been carried out for cobaltite thin films and nickelate single crystals, and constitute the first of their kind, particularly for the single crystals in which each crystallographic orientation is independently studied.

The pioneering work described above is expected to have a great impact on the understanding of the surface chemistry, surface properties and their relationship with the performance of these cathode materials. This new knowledge will greatly help to find new materials and to optimize the working conditions for improved performance not only of SOFC, but also of electrolysers, oxygen permeation membranes, gas sensors, etc