Experimental report

13/04/2016

Proposal: 5-25-233 **Council:** 4/2014

Title: In situ investigation of A-site order/disorder phase transition induced by an electric field in NdBaCo2O5, a promising cathode material for

Research area: Chemistry

This proposal is a new proposal

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Samples: NdBaCo2O5

Instrument	Requested days	Allocated days	From	To
D20	3	3	11/05/2015	15/05/2015

Abstract:

In situ neutron diffraction under electric field will be used to explore the phase transition transforming the A-site ordered tetragonal structure of NdBaCo2O5+d (a promising cathode material for SOFC) into a disordered cubic structure. Such experiments on LnBaCo2O5+d perovskites have not been investigated by diffraction techniques so far. The impact of the phase transition induced by the electric-field on the diffusion pathways of the O2- ions will be studied by means of the Maximum Entropy Method (MEM) analysis of the isothermal data collected on cooling under electric field combined to Molecular Dynamics calculations aiming to understand the role of A-site order/disorder phenomena on the oxygen diffusion process in a technologically important family of materials. The need for neutron diffraction lies in the sensitivity to the changes in the oxygen content induced by temperature and electric field. D20 will be used in its high take-off angle of 118° giving a wavelength of 1.3594 Å. Isothermal data will be collected at 100 °C intervals on cooling from 800 °C to room temperature.

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Experimental report for the experiment N° 5-25-233
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The purpose of the experiment was to investigate the crystal structure while measuring the electrical conductivity of a technologically important member of solid oxide fuel cell (SOFC) cathode materials, namely, $NdBaCo_2O_{5+\delta}$. We aimed to check for a structural phase transition induced by the electrical field applied on the sample and explore the dependence of such a phase transition on the intensity of the electrical field and temperature.

The experiment was carried out on the D20 very high intensity neutron 2-axis diffractometer. A thin $NdBaCo_2O_{5+\delta}$ dense bar was loaded in the quartz tube in the standard vanadium furnace. Electrical conductivity was measured in air with a dc four-probe method with Pt contacts on a bar of approximate dimension of 7 mm × 7 mm × 4 mm. Combined Neutron diffraction and electrical measurements were performed on heating in air at 200 °C intervals from 200 to 800 °C. A constant value of current (adjusted depending on the voltage measured) was applied. The samples were held for between 3 and 6 h at each temperature to allow for stabilization of the voltage response and ensure that chemical equilibrium (e.g. oxygen concentration) has been reached. After the measurement the current is switched off and another temperature was set, hence the current was applied only during the actual measurements

The feasibility of such experiment on D20 has been demonstrated. However, optimal combined electrical/neutron diffraction data require new sample environments to be developed. We are currently addressing this need working closely with staff at ILL and the LEPMI/Grenoble. The new environment will then be commissioned in a series of high profile neutron studies on systems synthesised at the University of Rennes to monitor electrical-field induced structural changes which are expected to play a key role in understanding conduction mechanisms in systems of interest. This will ultimately lead to a better understanding of the structure of various materials which may play a crucial part in future energy applications.