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Exploring oxygen diffusion mechanisms of Pr2NiO4+δ as a function of oxygen partial pressure at high temperature via single crystal neutron diffraction

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The development of new oxide materials for high energy conversion devices continues to be an area of strong interest. Oxides displaying nonstoichiometry due to Oxygen interstitial species have become one of the most promising alternatives in this field of study [1].

The aim of this project is to study the oxygen diffusion mechanisms of Pr2NiO4+δ as a function of the oxygen partial pressure by means of high resolution single crystal neutron diffraction. With this new perspective, one can expect to explore both the structural changes during the orthorhombic to tetragonal phase transition and the superstructure reflections that have been already observed to appear in this compound in previous high brilliance X-ray measurements [2-6].

This will be achieved by realizing comparative studies of the diffraction patterns obtained when increasing the temperature in atmospheric air conditions and after exposing the sample to a vacuum environment, studying the maximum and minimum apical Oxygen displacements. After this measurement, the atmosphere surrounding the sample will be controlled by means of a gas mixture of Argon and Oxygen allowing the study of the oxidation state inside the structure. Finally, pure Oxygen will be introduced to analyze the changes with maximum Oxygen content. Once finished, data refinement methods will be carried out and maximum entropy modelling will be fulfilled thanks to MaxEnt.

Due to the complexity of the experiment, a dedicated furnace has been constructed together with the gas system that will be implemented. Theoretical models have been done using SolidWorks and Comsol software simplifying the whole process. Once the fabrication process was completed, testing and safety procedures were hold in order to be able to perform the experiment.

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