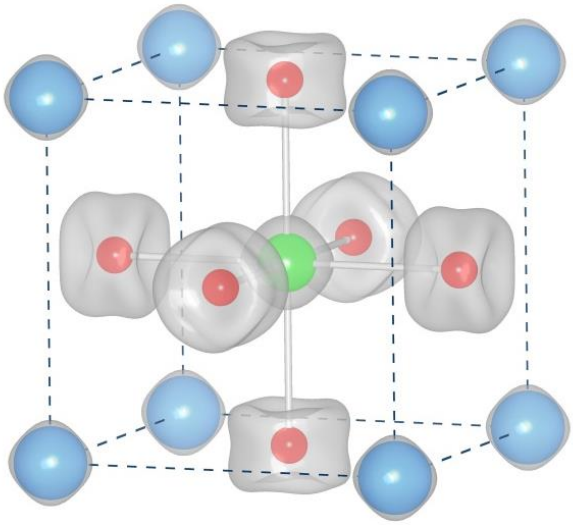
Structural features of a new oxygen deficient perovskite Sr_2ScGaO_5, a promising oxygen ion conductor at moderate temperature

Monica Ceretti, PhD Habil, Institut
Charles Gerhardt Montpellier
Montpellier, FRANCE

Oxygen ion conductors are materials of major interest for a series of application in the area of solid state ionics (fuel cells, batteries, electrodes, sensors, catalysts, etc…). In this respect oxides with brownmillerite type structure ($A_2BB'O_5$), have attracted much attention, especially as they show oxygen ion mobility down to ambient temperature. This mobility is a result of a phonon assisted diffusion mechanism, based on a dynamic oxygen disorder scenario of the infinite BO4 chains [1, 2].

Brownmillerite type frameworks containing B-cations with saturated or empty electron shells (d^0 or d^{10} configurations) present a special case, as they impose a fixed oxygen stoichiometry, making them good candidates to study oxygen diffusion mechanisms on a microscopic level. In this context, we have synthesized a new phase Sr_2ScGaO_5, having pure oxygen ion conductivity. Depending on the synthesis route, it shows two polymorphs: orthorhombic Brownmillerite type structure or an oxygen deficient cubic perovskite structure. When synthesizing Sr_2ScGaO_5 by classical solid state reaction at 1200°C, the thermodynamically stable phase obtained shows the brownmillerite framework [3]. Heating at higher temperature, it shows a phase transition to the cubic perovskite structure completed at 1500°C, associated with improved oxygen ion conduction [4]. Since the cubic symmetry can be maintained down to ambient temperature, we were able to grow high quality single crystal of the cubic phase [5].

We report here on a combination of characterization on the brownmillerite as well on the cubic Sr_2ScGaO_5. High-resolution structure analysis has been performed using X-rays (synchrotron and laboratory) and neutron diffraction methods, combined with NMR analysis for local environment [3]. In particular, single crystal neutron diffraction with subsequent analysis of the nuclear scattering density by the Maximum Entropy Method has been performed in order to describe in more detail oxygen displacement factors and associated diffusion pathways [5]. To better understand the oxygen mobility mechanisms, these studies were complemented by Raman and impedance spectroscopy.



Nuclear scattering density (in grey) of the Sr_2ScGaO_5 obtained at room temperature from neutron single crystal diffraction and subsequent Maximum Entropy reconstruction. The preovskite unit cell and the (Sc/Ga)O6 octahedra are outlined. While isotropic displacements are found for Sr and (Sc/Ga), oxygen atoms (in red) show an anisotropic disk shape distribution.

Recent Publications:

1. Paulus W. *et al.* (2008) Lattice Dynamics To Trigger Low Temperature Oxygen Mobility in Solid Oxide Ion Conductors. Journal of the American Chemical Society, 130(47): p. 16080-16085.
2. Ceretti M. *et al.* (2015) Low temperature oxygen diffusion mechanisms in $Nd_2NiO_{4+\delta}$ and $Pr_2NiO_{4+\delta}$ via large anharmonic displacements, explored by single crystal neutron diffraction. Journal of Materials Chemistry A, 3(42): p. 21140-21148.
3. Corallini S. *et al.*. (2015) One-Dimensional Oxygen Diffusion Mechanism in Sr_2ScGaO_5 Electrolyte Explored by Neutron and Synchrotron Diffraction, ^{17}O NMR, and Density Functional Theory Calculations. The Journal of Physical Chemistry C, 119(21): p. 11447-11458.
4. Ceretti M. *et al.* (2016) Influence of Phase Transformations on Crystal Growth of Stoichiometric Brownmillerite Oxides: Sr_2ScGaO_5 and Ca_2Fe2O_5. Crystals, 6(11): p. 146.
5. Corallini S. *et al.* (2017) Cubic Sr_2ScGaO_5 Perovskite: Structural Stability, Oxygen Defect Structure, and Ion Conductivity Explored on Single Crystals. Inorganic Chemistry, 56(5): p. 2977-2984..



Biography:

Monica Ceretti has an experitse in neutron diffraction for crystal structural studies. After 14 years at the Laboratoire Léon Brillouin (Saclay, France) as scientific responsible of a neutron diffractometer, she first moved to the University of Rennes and then in Montpellier (chemistry department), where she is in charge for structural studies of correlated oxides by neutron and X-ray diffraction. Member of several panels for proposals review at large scale facilities (at the ILL in the past and now at FRM2) in the crystallography committees, she is involved in training activities in neutron scattering for structural studies in the frame of master courses as well as in specialized schools.

Email: monica.ceretti@umontpellier.fr