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Structural complexity and O2- ordering in Pr2-xSrxNiO4+δ studied by single crystal neutron and x-ray diffraction

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Ruddlesden-popper phases and especially those with K2NiF4-type structure, are of particular interest, as they exhibit high ionic and electronic conductivity already at moderate temperatures. They show a rather wide range of oxygen non-stoichiometric and are able to accommodate extra oxygen on interstitial lattice sites. Hole doping in Pr2NiO4, either by substituting Pr with Sr cations or by O2- ion intercalation on interstitial lattice sites modifies the structural (ordering of O2- ions) and electronic ordering in Pr2-xSrxNiO4+δ. Contrary to Sr-doping a high oxygen doping level induces a special lattice dynamics, allowing the apical oxygen atoms to easily move to vacant interstitial sites on a shallow energy diffusion pathway. We evidenced by high resolution neutron single crystal diffraction, large displacements of the apical oxygen atoms, resulting in an phonon assisted diffusion mechanism, activated at already moderate temperatures [1,2]. The orthorhombic/tetragonal phase transition at 360°C induces an anharmonic Debye Waller behavior of the Pr2O2 rock salt layer separated by NiO-layers showing a normal displacement behavior with T.

Hole doping of Pr2NiO4 by oxygen insertion and/or Pr/Sr substitution, results in the formation of complex superstructures, related to charge and/or oxygen ordering. We report here on the influence of x, δ and T for Pr2-xSrxNiO4+δ, analyzed with X-ray and neutron diffraction studies.

Reference:
[1] M. Ceretti, O. Wahyudi, A. Cousson, A. Villesuzanne, M. Meven, B. Pedersen, J. M. Bassat and W. Paulus, J. Mater Chem. A, 2015.
[2] O. Wahyudi, M. Ceretti, I. Weill, A. Cousson, F. Weill, M. Meven, M. Guerre, A. Villesuzanne, J.-M. Bassat and W. Paulus, CrystEngComm, 2015.

Author: Mr DUTTA, Rajesh (ICMCB, UPR 9048, University Bordeaux, 33600 Pessac, France / Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France)

Co-authors: Dr VILLESUZANNE, Antoine (ICMCB, UPR 9048, University Bordeaux, 33600 Pessac, France); Mr MAITY, Avishek (Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France); Dr MEVEN, Martin (Institut für Kristallographie, RWTH Aachen University / FZ Jülich GmbH, Jülich Centre for Neutron Science JCNS, 85747 Garching, Germany); Dr CERETTI, Monica (Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France); Prof. PAULUS, Werner (Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France)

Presenter: Mr DUTTA, Rajesh (ICMCB, UPR 9048, University Bordeaux, 33600 Pessac, France / Institut Charles Gerhardt, UMR 5253, CNRS-University Montpellier, 34095 Montpellier, France)

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