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Non-stoichiometric transition metal oxides: exploring changes of structures and valance states by in situ neutron and synchrotron radiation.

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Perovskite type oxides exhibiting ionic or mixed electronic/ionic conductivity are of considerable interest for potential application e.g. solid oxide fuel cells, battery electrodes and sensor materials. $SrFeO_{2.5+x}$ is an important candidate for this type of oxides. A specific lattice dynamics involving low energy phonon modes has been recently identified to be at the origin of high oxygen ion mobility already at low temperature [1].

Over the oxygen composition of $0 \leq x \leq 0.5$, the $SrFeO_{2.5+x}$ system shows four distinct phases with x=0, 0.25, 0.375 and 0.5. The starting phase $SrFeO_{2.5}$ has a oxygen deficient Brownmillerite type structure with 12-fold twinning and shows G-type anti-ferromagnetism where as the last candidate in this series $SrFeO_3$ which can be obtained by electrochemical oxidation has a cubic Perovskite structure showing helimagnetism. The system $SrFeO_{2.5+x}$ has been extensively studied for last four decades and still it is of high interest because of the inherent complexity present in this system. Different space groups have been assigned to $SrFeO_{2.5}$ e.g. Imma [2], Pbma [3] etc. but still they are highly debated.

The aim of this master thesis is a detailed structure analysis of antiferromagnetic 12-fold twinned $SrFeO_{2.5}$ single crystals using synchrotron and neutron diffraction and also to explore the phase diagram by following the electrochemically controlled oxygen intercalation reaction into $SrFeO_{2.5}$ forming $SrFeO_3$ by in situ single crystal synchrotron diffraction, performed in a specifically designed electrochemical cell.

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[2] Hodges, J.P.; Short, S.; Jorgensen, J. D.; Journal of Solid State Chemistry, 2000, 151, 190-209.
[3] Auckett, J. E.; Studer A. J.; Sharma, N.; Ling, C. D.; Solid State Ionics, 2012, 225, 432–436.

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