

$\text{SrCo}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$: Structure Property Relation

S. Marik^a, C. Madhu^a, O. Toulemonde^a

^a CNRS, Université de Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

The family of perovskite related Sr and Co containing compounds has received considerable attention as oxygen-permeating membranes, sensors, or cathodes for Solid oxide fuel cell (SOFC) because of their high oxygen permeability values [1]. $\text{SrCoO}_{3-\delta}$ phases with 3C-like crystal structures are presented as mixed conductors with very high oxygen permeability [2]. On the other hand, the $\text{SrCoO}_{3-\delta}$ samples with 2H-like hexagonal structures at room temperature (RT) have shown to be almost non-oxygen permeable [3].

Recently, A-site ordered 314 phase with composition $\text{Sr}_{0.7}\text{Y}_{0.3}\text{CoO}_{2.65}$ [4] has been reported to crystallize with a novel oxygen vacancy ordering that gives a tetragonal structure (space group $I4/mmm$), with $2a_p \times 2a_p \times 4a_p$ unit-cell, where a_p is the parameter of the cubic perovskite unit cell. At the same time, the compound is a mixed oxide-ion/electronic conductor exhibiting good activity for the oxygen-reduction reaction, which makes it a competitive cathode material for an intermediate-temperature (IT) SOFC [5].

The aim of the present work is to stabilize the Sr-Co-O system in a 314-type oxygen vacancy ordered structure without A-site ordering to provide the high oxygen mobility within the oxygen deficient plane, which will be adequate for the cathode of an IT-SOFC. With this in mind, we have substituted Co in the $\text{SrCoO}_{3-\delta}$ system by Fe. Here, we present and discuss a systematic and detailed composition-structure-property relation for the $\text{SrCo}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ samples. The investigation on the evolution of crystal structures with Fe substitution and their structural determination is carried out using the X-ray and Neutron powder diffraction patterns. Three different oxygen vacancy ordered structure is observed for different Fe substitution and the driving forces to stabilize the 314-type oxygen vacancy ordered structure without A-site ordering and their relevance for the cathode of an intermediate temperature SOFC will be discussed.

[1] J. Fleig, J. Maier, J. Eur. Ceram. Soc. 24 (2004) 1343.

[2] Z. Q. Deng, W. S. Wang, W. Liu, C. S. Chen, J. Solid State Chem. 179 (2006) 362.

[3] H. Kruidhof, H. J. M. Bouwmeester, R. H. E. V. Doorn, A. Burggraaf, J. Solid State Ionics 63-65 (1993) 816.

[4] S. Ya. Istomin, J. Grins, G. Svensson, O. A. Drozhzhin, V. L. Kozhevnikov, E. V. Antipov, J. P. Attfield, Chem. Mater. 15 (2003) 4012.

[5] Yan Li, Young N. Kim, Jinguang Cheng, José A. Alonso, Zhiwei Hu, Yi-Ying Chin, Tsuyoshi Takami, Maria T. Fernández-Díaz, Hong-Ji Lin, Chien-Te Chen, Liu H. Tjeng, Arumugam Manthiram, and John B. Goodenough, Chem. Mater. 23 (22) (2011) 5037-5044.