

**MS13-P12** **Crystal and twin structure in LSGMn crystals**  
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Solid oxide fuel cells (SOFC) are most promising energy sources for appropriate applications. Though solid oxide fuel cells have many physical and chemical advantages, the SOFC-technology has serious difficulties to develop inexpensive materials and production techniques. LaGaO<sub>3</sub> doped with Sr and Mn (LSGMn) is currently considered as a prospective anode material in SOFC, especially for intermediate-temperature-SOFC with LaGaO<sub>3</sub> doped with Sr and Mg (LSGM) as solid electrolyte [1, 2]. This work presents results of the structure investigations of La<sub>0.95</sub>Sr<sub>0.05</sub>Ga<sub>0.95</sub>Mn<sub>0.05</sub>O<sub>3-x</sub> (LSGMn-05) and studies its twin structures in the ferroelastic phases.

The evolution of the crystal structure of the perovskite-type LSGMn-05 crystal in the temperature range 298-1173 K has been studied by means of powder diffraction technique using synchrotron radiation (beamline B2, HASYLAB, DESY). *In situ* high temperature powder diffraction experiments were performed in a STOE capillary furnace in Debye-Scherrer geometry using an Image Plate detector. Crystallographic data refinements were performed by the full profile Rietveld method using the WinCSD program package. The ferroelastic domain structure of the LSGMn-05 crystal was investigated by the Laue method. Experiments were carried out at the F1 beamline at HASYLAB using a *Kappa*-diffractometer and a MAR CCD detector. Laue patterns were collected at distance 100 and 300 mm from specimen to detector at temperatures from 293 to 973 K using a gas-flow heating device.

The analysis of the obtained diffraction data at room temperature showed orthorhombic *Pbnm* structure of LSGMn-05. At about 340 K a first order phase transition from the orthorhombic to rhombohedral *R $\bar{3}c$*  structure was detected. From the extrapolation of the *c/a* parameter ratio of the rhombohedral phase a continuous phase transitions from the rhombohedral to a cubic structure in the LSGMn are predicted to occur near 2063 K.

Analysis of the Laue patterns showed that the LSGMn-05 crystal has four domains configuration of twin structure in the rhombohedral phase. The domains are interconnected by twin walls – i.e. mirror planes with Miller indexes (211), (101) and (110). Due to crossing of these walls chevron-like domain patterns are formed, which result from the relaxation of the structural strain caused by the phase transition cubic → rhombohedral.

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**MS13-P13** **Structure and morphology of nanosized Ce<sub>0.8</sub>Gd<sub>0.2</sub>O<sub>1.9</sub>/Ni infiltrate in a ceramic anode of a solid oxide fuel cell**  
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CeO<sub>2</sub>-based materials have received intensive attention as they have a lot of important physical, chemical and electrochemical properties [1]. Recently, Gd-doped CeO<sub>2</sub> (CGO)/Ni infiltrate was found to exhibit good ionic and electronic conductivity, and is therefore utilized as an effective electrocatalyst to greatly enhance the electrocatalytic activity for fuel oxidation in solid oxide fuel cells (SOFCs) [2,3]. In order to understand the improved performances and possible degradation mechanisms, it is critical to perform a full characterisation of both structure and morphology of the CGO/Ni infiltrate. In this work, the structure and morphology of Ce<sub>0.8</sub>Gd<sub>0.2</sub>O<sub>1.9</sub>/Ni (CGO/Ni) nanoparticles infiltrated into a backbone ceramic anode (a composite of doped strontium titanate and yttria stabilised zirconia) of a symmetric cell was investigated by using a JEM-3000F microscope equipped with a field-emission gun, operated at 300 kV. High-resolution transmission electron microscopy analysis of the infiltrate reveals that the nanoparticle size is mostly in the ~5 nm range. By indexing the continuous electron diffraction rings, the four main crystal planes of CGO, (111), (200), (220) and (311) were well identified for the nanoparticles. The CGO/Ni infiltrate appears to be mainly as a typical fluorite structure, where Ni may be well dispersed in the lattice of CGO, either substituting Ce<sup>4+</sup>/Gd<sup>3+</sup> or at interstitial sites as there is a large difference of ionic radius [4] between Ni<sup>2+</sup> and Ce<sup>4+</sup>/Gd<sup>3+</sup> [5]. Consistent with the aforementioned phase analysis, information was also obtained for chemical composition of the infiltrate. In scanning transmission electron microscopy mode, the energy dispersive X-ray spectroscopy (EDX) elemental maps of the infiltrate reveal that cerium, gadolinium and nickel have a very similar distribution in the whole region; EDX line scan profiles show that the line profile of nickel is correlated closely with those of cerium and gadolinium, at each particular location. In summary, considering the combination of phase structure and chemical composition, the infiltrated CGO/Ni precursors appear to mainly form a fluorite structure with particle sizes in the ~5 nm range after calcinations. Results such as this can prove important to elucidate the nature of the processes-involved CGO/Ni electrocatalyst in fuel cell anodes.

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