Microstructure of $LaMO_3$ perovskites (M=Ni,Co,Fe)

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Perovskites have been a research topic of huge interest for a long time due to their variability in composition and crystal structures. Depending on these factors, they can display a wide range of material properties [1], which make them highly interesting for various applications. In order to enable a prediction of their material characteristics, it is essential to analyze the structure-property relationship by describing the crystal structures in detail.

In our research we have synthesized $LaMO_3$ perovskites with M=Ni,Co,Fe via incipient wetness impregnation of mesoporous carbon spheres and subsequent sintering [2]. The aim of this work is to describe the microstructure of our perovskites in detail and to set up a structural model deviating from the so far published ideal crystal structure if necessary. Analysis via transmission electron microscopy enabled the identification of Ruddlesden-Popper (RP) faults in the case of the $LaNiO_3$ sample. These [LaO]-[LaO] shear faults have been reported in the past to be present in $LaNiO_3$ thin films grown on various substrates [3, 4]. Based on that a Rietveld refinement of synchrotron powder diffraction data (beamline P02.1, PETRA III, DESY) was performed with a phase combination of the ideal crystal structure, space group R-3cH, and a stacking fault model based on its superstructure, space group Pm-3m (Fig. 1). This shows that large parts of our $LaNiO_3$ sample are still undistorted, while some areas show a significant amount of RP stacking faults. In addition, the local structure of the perovskites was investigated by neutron and synchrotron total scattering experiments and subsequent pair distribution function analysis, which supports the previously obtained results.

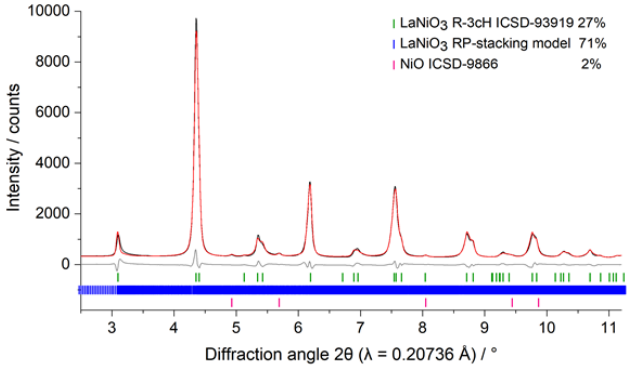

Fig. 1 Rietveld refinement plot of $LaNiO_3$ (r_{wp} 5.4) with the ideal crystal structure model a=b=5.4608(5)Å, c=13.144(2)Å, α=β=90°, γ=120°, space group R-3cH and with a crystal structure model containing RP-type faults stacked along the c-axis, a=b=3.8500(3)Å, α=β=γ=90°, space group P1, by-phase is NiO.

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