MS17 Total scattering studies and disorder

MS17-03

The local structure of oxygen deficient perovskite Sr_2ScGaO_5 polymorphs explored by total neutron scattering and EXAFS

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Abstract

Oxygen deficient perovskite oxides have been extensively investigated in the last decades because of their rich chemistry, structural complexity, interesting properties and applications, such as ionic conductors.[1-5] We have recently reported on oxygen diffusion mechanisms in a new oxygen deficient perovskite, Sr_2ScGaO_5 (SSGO), containing exclusively open or closed shell B-cations and fixed oxygen stoichiometry.[5-8] Depending on the synthesis route, it adapts two polymorphs: the orthorhombic brownmillerite (*I2mb*), or an oxygen deficient perovskite structure (*Pm-3m*). Once synthesized, both phases are surprisingly kinetically stable up to 1400°C, making them as a model system to study oxygen diffusion mechanisms6. We report here on a multi-technical approach to characterize structural changes as a function of temperature using X-ray and neutron diffraction techniques. To further investigate the local structure, neutron pair distribution function (PDF) analysis together with the extended X ray absorption fine structure (EXAFS) analysis were carried out on both SSGO polymorphs. Our studies confirm a 2nd order phase transition for SSGO with Brownmillerite framework, implying an order/disorder transition of the 1D (GaO_4) tetrahedral chains indicating dynamical switching activated above 300°C. For the oxygen deficient SSGO perovskite, oxygen vacancies do not show a statistical distribution but are correlated. From PDF analysis we clearly proof that on a local scale the brownmillerite type vacancy structure exists, suggesting that the average cubic perovskite framework is consisting of a complex microstructure. In addition to this, EXAFS first shell analysis, indicate for both polymorphs an identical local environment for the Ga atoms. Temperature dependent structure and local structure (PDF) analysis, combined with EXAFS spectroscopy, are discussed in terms of lattice dynamical aspects obtained from ^{17}O-NMR and Raman spectroscopy .

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Neutron G(r) refinements for the cubic SSGO