Anomalous Lattice Expansion of $Sm_{0.5}Pr_{0.5}FeO_3$ Derived From X-Ray Synchrotron Powder Diffraction Data

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Complex oxides with perovskite structure RFeO$_3$, where R are rare earth metals, represent an important class of functional materials. The RFeO$_3$ compounds are used in thermoelectric devices and solid oxide fuel cells, as membranes for partial oxidation of methane and oxygen cleaning, as catalysts for CO oxidation and decomposition of NO_x, and as sensory materials. Complementary, the interest in the rare earth ferrites is stimulated by their interesting fundamental physical properties, such as spin-reorientation transitions at 80–200 K and the para- to antiferomagnetic transitions at 620–750 K. Just recently, $SmFeO_3$ has attracted considerable attention due to its reported multiferroic properties above room temperature.

Mixed samarium-praseodymium ferrite $Sm_{0.5}Pr_{0.5}FeO_3$ was synthesized by conventional solid state reaction technique in air at 1473 K for 20 h. Lattice parameters at room temperature are in good agreement with the end members of the $SmFeO_3$–$PrFeO_3$ system, thus proving a formation of the continuous solid solution $Sm_{1-x}Pr_xFeO_3$. Thermal behaviour of the structure has been studied *in situ* in the temperature range of 298–1173 K by means of high-resolution X-ray synchrotron powder diffraction technique. Corresponding experiments were performed at synchrotron laboratory *HASYLAB/DESY* (Hamburg, Germany).

As it was established, $Sm_{0.5}Pr_{0.5}FeO_3$ remains orthorhombic in the whole temperature range investigated. No structural phase transitions were detected. However, strongly anisotropic anomalous lattice expansion is observed. The lattice parameters exhibit an anomalous kink around 670 K that is obviously indicative for magnetoelastic coupling at the magnetic ordering temperature T_N, similar to recently reported for $SmFeO_3$ [1].

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[1] C.-Y. Kuo, Y. Drees, M.T. Fernández-Díaz, L. Zhao, L. Vasylechko *et al.* k=0 magnetic structure and absence of ferroelectricity in $SmFeO_3$. *Phys. Rev. Letters* 113 (2014) 217203.