Crystal structure and magnetism in $Nd_{1-x}Sr_xFeO_3$ (0.1≦x≦0.9)

H. Nakatsugawa[1], Y. Kamatani[1], C.H. Hervoches[2]

[1]Yokohama National University, Japan,
[2]Nuclear Physics Institute, Řež, Czech Republic

hervoches@ujf.cas.cz

As in the smaller doping range ($0.0 \leq x \leq 0.5$) [1,2], $Nd_{1-x}Sr_xFeO_3$ adopts an orthorhombic (space group: Pnma) ABO_3 perovskite structure at room temperature, for all compositions within $0.1 \leq x \leq 0.9$.

Magnetization measurements from 5K to 700K show weak antiferromagnetic behaviour and paramagnetism following the typical Curie-Weiss law above 600K. Assuming that the spin state of the Fe site is (LS Fe^{3+}_y IS $Fe^{3+}_{1-y})_{1-x}$ LS Fe^{4+}_x, the ratio of intermediate spin (IS) Fe^{3+} gradually decreases as x increases, and it decreases rapidly when x≧0.6. This decrease in the ratio of IS Fe^{3+} with the increase in x is expected to show a large correlation with the relaxation of the FeO_6 octahedron distortion.

To clarify the correlation between the crystal structure and magnetic structure of $Nd_{1-x}Sr_xFeO_3$ ($0.1 \leq x \leq 0.9$) in more detail, powder neutron diffraction (PND) data of the $Nd_{1-x}Sr_xFeO_3$ ($0.1 \leq x \leq 0.9$) samples were collected at room temperature with the medium resolution neutron powder diffractometer (MEREDIT), part of the CANAM infrastructure, at the Nuclear Physics Institute, Czech Republic. All Rietveld refinements were carried out using the GSAS-II suite of programs [1].

It is confirmed that the FeO6 octahedron distortion is relaxed as x increases and approaches the crystal structure of the pseudo-cubic. Fig 1 shows the evolution of Fe-O-Fe angles with x in $Nd_{1-x}Sr_xFeO_3$ ($0.1 \leq x \leq 0.9$).

The materials present antiferromagnetic order, with magnetic moment of Fe decreasing from ~ 3.2 μB for x = 0.1 to ~0.2 μB for x = 0.9. With $0.1 \leq x \leq 0.4$, the magnetic spins are oriented in the c-axis direction (BNS Magnetic Space Group: Pn'ma'), while for $0.5 \leq x \leq 0.9$ they appear to be in the a-axis direction (BNS Magnetic Space Group: Pnma). The magnetic structures for $Nd_{0.9}Sr_{0.1}FeO_3$ and $Nd_{0.5}Sr_{0.5}FeO_3$ are shown in fig 2. Crystal and magnetic structures were drawn using VESTA [2].

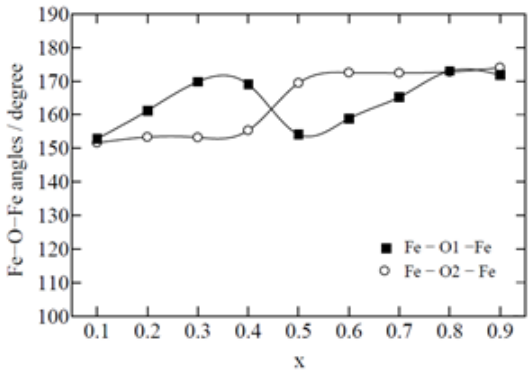

Figure 1. Evolution of Fe-O-Fe angles vs x.

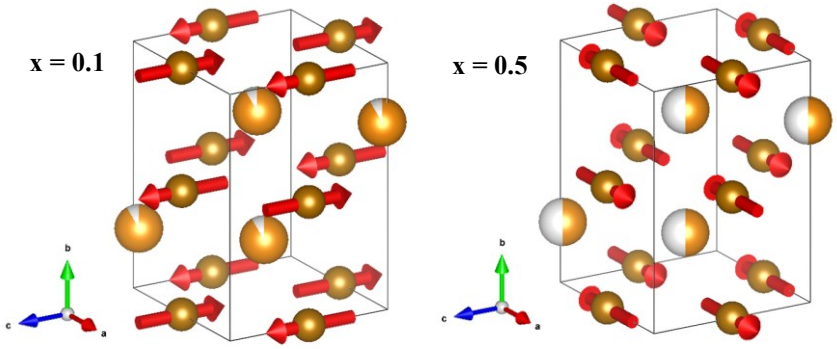

Figure 2. Magnetic structure of $Nd_{0.9}Sr_{0.1}FeO_3$ (x = 0.1) and $Nd_{0.5}Sr_{0.5}FeO_3$ (x = 0.5) at room temperature.

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