Structure and Physical Properties of *A*-site Layer-ordered/disordered Perovskites $NdBaFe_2O_6$ with Unusually High Valence $Fe^{3.5+}$

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A-site layer-ordered perovskites $RBaFe_2O_6$ (*R* = rare-earth metals) were recently found to have successive phase transitions. In the previous presentation, it was reported that the transitions were related to not only relieving of charge instability of unusually high valence $Fe^{3.5+}$ but also ionic radius of rare-earth metals. However, it has not been revealed the effect of *A*-site layer-ordering on the successive phase transitions of $RBaFe_2O_6$ although the behavior of phase transition depends on *A*-site order/disorder in similar perovskite compounds.[1] Then we tried to synthesize *A*-site disordered sample $Nd_{0.5}Ba_{0.5}FeO_3$ and compared its physical properties with those of *A*-site layer-ordered $NdBaFe_2O_6$.

A-site disordered sample was successfully synthesized by high-temperature solid state reaction with flowing O_2 gas while *A*-site layer-ordered sample was synthesized by ozone oxidation. Their crystal structures were determined by Rietveld refinement of Synchrotron X-ray Powder Diffraction data (Figure 1). Physical properties such as magnetic susceptibility of both samples were measured and the results suggested that *A*-site layer-ordering had an important role in the phase transitions of $NdBaFe_2O_6$ (Figure 2). We will discuss the effect of *A*-site layer-ordering on physical properties of $NdBaFe_2O_6$ and the possibility of causing phase transitions by cation-orderings in perovskite metal oxides.

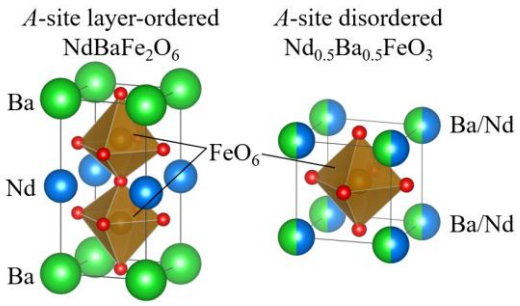

Figure 1 : Crystal structures of *A*-site layer-ordered/disordered $NdBaFe_2O_6$

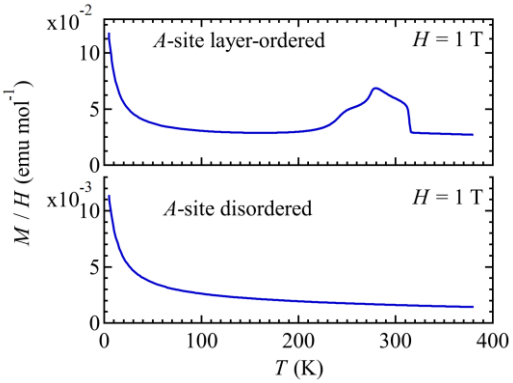

Figure 2 : Temperature-dependent magnetic susceptibility upon cooling

1) F. Denis Romero *et al.*, *Chem. Commun.*, **2019**, *55 (26)*,3690-3696