Powder Diffraction of Charge Disproportionate Perovskite and Layered Pervskite Oxides of $CaFeO_3$ and $Sr_3Fe_2O_{7-x}$

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"Charge disproportionation" is found only in pervskites and related oxides with Fe^{4+} system, is interesting phenomenon: $2Fe^{4+} \rightarrow Fe^{3+} + Fe^{5+}$. Mössbauer effects reveals charge disproportionation firstly in perovskite $CaFeO_3$ below 290 K [1, 2].

$CaFeO_3$ is slightly distorted into a class of orthorhombic perovskite. On the other hand, $SrFeO_3$ has cubic perovskite structure and no charge disproportionation is occuerd down to 4.2 K [3].

In the series of $Sr_{n+1}Fe_nO_{3n+1}$, Sr_2FeO_4 (n=1) with the K_2NiF_4 structure have two-dimensional linkage of FeO_6 whereas cubic $SrFeO_3$ (n→∞) has three-dimensional one. The $Sr_3Fe_2O_7$ (n=2) has a "layered" perovskite structure [4]. $Sr_3Fe_2O_7$ only displays charge disproportionation in these series [5].

$CaFeO_3$ are synthesized under 3 GPa and at 1273 K with $KClO_4$ as an oxidizer. Oxygen-deficient $Sr_3Fe_2O_{7-x}$ with $x \sim 0.3$ (sample #1) and $x \sim 0.2$ (#2) were used for this study. Final annealing conditions are 1173 K for 1 week in air for sample #1, and 723 K for 3.5 days in O_2 flow for #2.

Powder diffraction experiment was performed at BL02B1 with bending magnet in SPring-8. The storage ring was operated at 8 GeV. The incident beam with photon energy of 24.8 KeV (0.5 Å) was monochromatized by two set of Si(311), and collimated by a hole with 0.5 mm in diameter. All samples were charged in a quartz tube with 0.3 mm in diameter. The tube was set on the phi axis and rotating during the measuerment to eliminate the effect of prefered orienation. Diffraction pattern was recorded in a imaging plate on a film cassette prepared for the Weissenberg method.

Since diffraction data are converted to one-dimensional data in *incorrect* way, further conversions are required, which are now in progress.
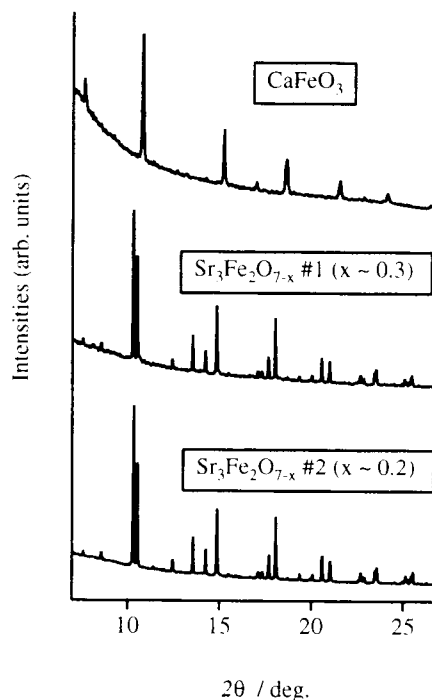

Fig.1. Powder diffraction patterns of $CaFeO_3$, $Sr_3Fe_2O_{7-x}$ #1, and #2 at $\lambda = 0.5$ Å

References
[1] M. Takano *et al.*, Mater. Res. Bull. **12** (1977) 923.
[2] S. Nasu *et al.*, Hyp. Int. **70** (1992) 1063.
[3] J. B. MacChesney *et al.* J. Chem. Phys. **43** (1965) 1907.
[4] S. E. Dann, M. T. Weller and D. B. Currie, J. Solid State Chem. **97** (1993) 179.
[5] S. E. Dann, M. T. Weller, D. B. Currie, M. F. Thomas and A. D. Al-Rawwas, J. Mater. Chem. **3** (1993) 1231.