Poster Presentation

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Synthesis and crystal structure of Sr2MnGaO5-dFx, layered oxyfluorides

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Sr2MnGaO5 brownmillerite has an interesting structure. In this compound, MnO6 octahedra and GaO4 tetrahedra are ordered along c-axis. The MnO6 octahedra are deformed due to Jahn-Teller effect with four short equatorial Mn-O distances and two long apical one. Oxygen vacancies in the GaO layer provide distorted tetrahedral coordination for the Ga cation. The oxide and/or fluoride ions are introduced into the vacancies in GaO layer. The synthesis of Sr2MnGaO4.78F1.22 using XeF2 as a fluorinating agent is reported, while the small amount SrF2 impurity is contained[1]. On the other hand, low temperature fluorination using polyvinylidenefluoride (PVDF) is powerful method for the synthesis of oxyfluoides from brownmillerite[2]. In this study, we synthesize the Sr2MnGaO5-dFx (x=0.5, 1.0, 1.5, 2.0) using PVDF and investigate the variation of crystal structure with x. Sr2MnGaO5 brownmillerites were prepared sold state reaction method. Starting materials were SrCO3, Mn2O3 and Ga2O3. The mixture was heated twice in Ar at 1300°C for 72h. For the preparation of Sr2MnGaO5-dFx (x=0.5, 1.0, 1.5, 2.0), stoichiometric amounts of Sr2MnGaO5 brownmillerite and PVDF were ground and the mixture were heated in N2 at 400°C for 8h. And then, the as prepared materials were subsequently heated in O2 at 400°C for 8h. The Sr2MnGaO5-dFx were obtained without impurities. As shown in Fig., the orthorhombic distortion reduced with the increase in x. The X-ray diffraction data of Sr2MnGaO5-dF1.0 could be refined on the structure model belonging the space group Icmm. the bond valence sum of Ga3+ calculated from Ga-O bond length indicates that the fluoride ions are introduced into GaO layer preferentially. The measurements of magnetic properties for Sr2MnGaO5-dFx are in progress.

[1] *A. M. Alekseeva et al., J. Sold State Chem., 177 (2004) 731.,* ***[2]*** *F. J. Berry et al., J. Sold State Chem., 184 (2011) 1361.*

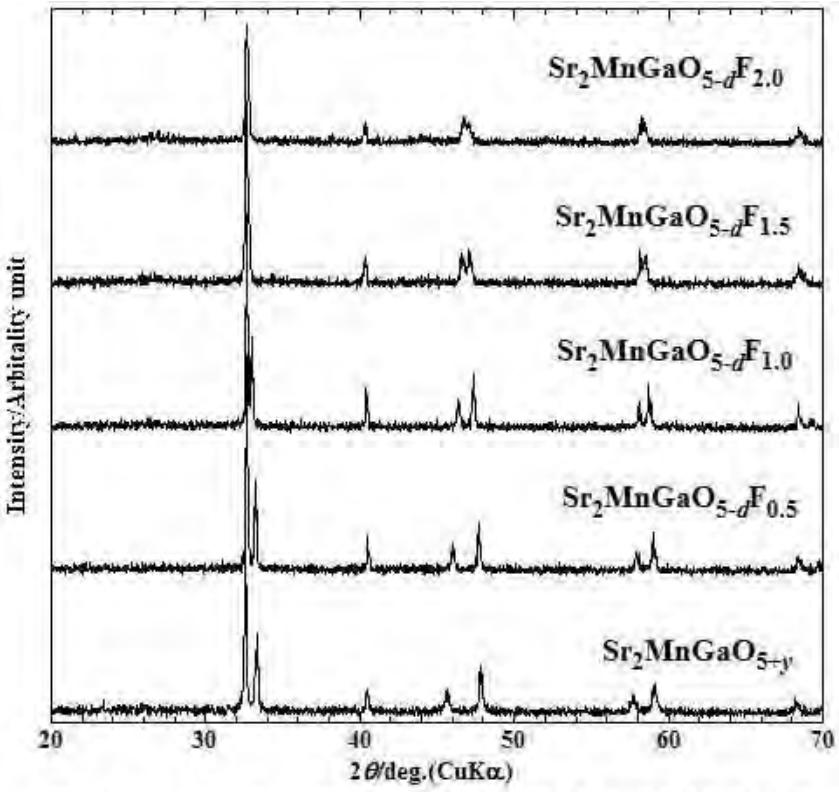

Fig.1 X-ray diffraction patterns for $Sr_2MnGaO_{5-d}F_x$ (x=0.5, 1.0, 1.5, 2.0)

Keywords: crystal structure, oxyfluorides, bond valence sum