Poster Presentation

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Crystal structure analysis of layered oxides $In_3V_2MO_{10}$(M=Al,Cr,Ga)

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Transparent conducting oxides represented by InGaZnO4(IGZO) [1] are very important practical materials for the displays and electric devices today. Many kinds of materials are synthesized by substituting atoms to date. For example, In3FeTi2O10(IFTO) has monoclinic and orthorhombic structures by the synthesis condition [2]. They have different stacking of InO6 octahedron layer and (Fe,Ti)-O polyhedron layer. These materials have layered structures similar to delafossite characterized by the InO6 octahedron layers. In the present study, crystal structures of novel materials In3V2MO10(M=Al,Cr,Ga) were investigated by synchrotron powder diffraction.

Powder samples were synthesized by a solid-state reaction method mixing appropriate amounts of In2O3, VO2 and M2O3 powder. The diffraction measurements were carried out using a large Debye-Scherrer camera at the beamline BL02B2, SPring-8. An imaging plate was used as a detector to measure the high counting statistic diffraction data. Some unit cells searched by the indexing software have fairly large cell parameters and we investigated fundamental structures of these materials as the first step of the structure determination. By indexing and consideration of symmetry, space groups were determined to be Cmcm for In3V2AlO10, R-3 for In3V2CrO10 and C2/m for In3V2GaO10. Using the previously reported structures as references, initial structures model were constructed and Rietveld refinements were carried out. In In3V2GaO10, the initial structure model was formed in reference with IFTO structure. However the fitting between the observed and calculated profiles was not sufficient in Rietveld analysis. Oxygen atom positions in the layer of (V,Ga)-O polyhedron layer were reinvestigated by the omit-MEM(maximum entropy method) charge density analysis. In the revised model, oxygen positions changed and oxygen atoms were suggested to have disordered arrangement within the atomic layer.

In comparing the crystal structures of three materials, the InO6 polyhedron layer is identical and the stacking of the InO6 and (V,M)-O polyhedron layers is different. It was also found that the oxygen arrangement which corresponds to that of (V,M)-O polyhedron has characteristic differences. The accurate crystal structure analyses including super-lattice reflections are needed for further understanding of the principles of structure formation in these materials.

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