

powder diffraction, structure-properties relationship

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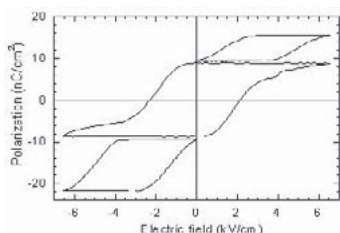
Discovery of polarization flop and ferrielectric character of multiferroic RMn_2O_5

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Rare-earth (R) manganese oxides of the form RMn_2O_5 are known as multiferroic materials which exhibit colossal magnetoelectric effects because of magnetic frustration and dielectric properties strongly coupling with magnetic ordering. However, the origin of the ferroelectricity of RMn_2O_5 is not yet clear. We have studied the relationship between dielectric properties and magnetic ordering of RMn_2O_5 especially by simultaneous measurements of the electric polarization and permittivity under neutron diffraction, and discovered several new facts. It is believed that the ferroelectricity of RMn_2O_5 appears only along the *b*-axis. But we discovered that the polarization of TmMn_2O_5 flops from the *b*-axis to the *a*-axis below about 5 K, which is attributed to a magnetic phase transition in an incommensurate magnetic phase. According to a structure analysis, RMn_2O_5 may be ferrielectric.

Actually both ferroelectric and antiferroelectric hysteresis loops of ErMn_2O_5 are observed as the figure at 35.4 K, in a commensurate magnetic phase. These loops can be obtained by a Sawyer-Tower circuit with a new technique, the double-wave method.



Keywords: ferroelectrics, magnetic frustration, neutron diffraction

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Structure and magnetic property of one-dim. chain complex: $\text{M}^{\text{II}}(\mu\text{-bpt})(\mu\text{-COOC}_5\text{H}_4\text{N})\cdot\text{H}_2\text{O}$ (M=Mn, Fe)

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The one dimensional chain complex, $\text{M}^{\text{II}}(\mu\text{-bpt})(\mu\text{-COOC}_5\text{H}_4\text{N})\cdot\text{H}_2\text{O}$ (M=Mn, Fe), with the metal centers connected each other with bpt and isonicotinic acid forms an infinite chain along a screw axis 4₁. It is synthesized by solvo-thermal synthesis and the structure is characterized by single crystal x-ray diffraction. The complex is crystallized in tetragonal space group *I*4₁/*a* with cell parameters of *a* = *b* = 21.5910(2), *c* = 15.2330(3) Å. It is iso-structure for both metal ions. Fe(II) is octahedrally coordinated by four nitrogen of bpt and two oxygen of isonicotinic acid, $[\text{FeN}_4\text{O}_2]$. The bond lengths of Fe-N are 2.331(1) Å, 2.130(1) Å, 2.233(1) Å, 2.126(1) Å and of

Fe-O are 2.057(1) Å, 2.093(1) Å at 300 K; which are typical bond lengths of FeII at its high spin state. However, this Fe chain complex displays distinct ferromagnetic interaction between the FeII centers. The hydrogen bonds between water molecules and the ligands may play important role on the inter-chain interactions. On the contrary, the Mn(II) complex shows typical paramagnetic character with antiferromagnetic interaction at low temperature, even the structure is exactly the same as that of Fe chain complex. The detail structure of the chain complexes and the comparison on the magnetic property of the two metal chain complexes will be presented.

Keywords: inorganic materials, one-dimensional structures, magnetic properties

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Structural change of cordierite by substitution Ni for Mg bringing high *Q* on millimeterwave ceramics

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Cordierite ($\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}$) is a candidate for millimeterwave dielectrics because of the low dielectric constant of 6.19. This study has been focused on the affects of substitution Ni for Mg in octahedron. In the case of octahedron substitution, the quality factor *Q* of the Ni-substituted analogy with single phase was improved from 39900 to 90600 GHz. The origin of improvement of *Q* comes from changing to the high symmetry which is from orthorhombic to hexagonal. Here, cordierite with orthorhombic system *Cccm* (No.66) transforms to indiarite with hexagonal system *P6/mcc* (No.192). It is confirmed based on the crystal structure obtained by Rietveld method that configuration of $\text{Si}_4\text{Al}_2\text{O}_{18}$ ring changes to hexagonal ring from distorted ring according to the substitution Ni for Mg. The volumes and covalencies of SiO_4 and AlO_4 tetrahedra also change to same size according the substitution. The crystal structure tends to become higher symmetry hexagonal ring with accompanying Si-Al disordering. In this case, contribution of high symmetry for *Q* might be greater than that of ordering.

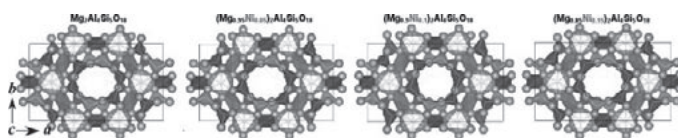


Fig. 1 Structural change on cordierite substituted Ni for Mg.

Keywords: microwave materials, indiarite, order-disorder structure

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On-line symmetry-mode analysis of any ferroic structure

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We report the addition to the Bilbao Crystallographic Server (www.cryst.ehu.es) of a new tool that can perform the symmetry