distribution maps obtained from the maximum entropy method (MEM) describe that 13.4 % of protons exist at inter-layer space. Proton diffusion constants were estimated as $1.9(1) \times 10^{-10}$ m^2/s at 393 K and $2.1(3) \times 10^{-10}$ m^2/s at 413 K respectively. The structural change corresponds to a rotational mode of SeO$_4$ tetrahedra, which is led from the group theoretical analysis from *R3m* to *C2/c*. A diffusive spectrum was observed around 0 meV at the L-point (0.5 2 0) above T_C as an over dumped phonon mode. The rotational mode of SeO$_4$ tetrahedra drives the improper ferroelastic phase transition, and assists the disconnection and reconstruction of hydrogen bonds in the high temperature phase.

Keywords: neutron diffraction elastic and inelastic, proton conductivity, phase transitions

P11.12.60

X-ray diffuse scattering and a local structure of (CH$_3$)$_4$NCdCl$_3$ (TMCC) and related compounds

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A local structure of TMCC has been determined by configurational-bias reverse Monte Carlo method basing on X-ray diffuse scattering data. Two phases have been analysed and refined: phase I at 293 K, P6_3/*m* space group, $a = 0.9139(1)$ nm, $c = 0.6723(1)$ nm, and phase I' at 410 K, $P6_3$/*mmc* space group, $a = 0.9235(1)$ nm, $c = 0.6742(1)$ nm. A model dividing CdCl$_6$ octahedra chains into elementary bricks has been implemented in order to take into account coupling between orientation of TMA molecules and local deformations of the octahedra chains. The resulting structures contain the subchains of CdCl$_6$ octahedra shifted longitudinally away from their average positions. Their lengths show the Poisson-like distribution with an average value of about 6 unit cells. X-ray diffuse scattering effects observed on the *hk*0 plane require the existence of the transverse subchain displacements. Additional transversal correlation between longitudinal shifts of the subchains is needed to explain weak modulation effects and diffuse streaks observed on the planes perpendicular to *c**.

Keywords: disordered systems, diffuse scattering, reverse Monte Carlo

P11.12.61

Magnetoelastic effects in BiMn$_2$O$_5$: A high-resolution synchrotron x-ray diffraction study

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Multiferroic materials with coexisting (anti)ferromagnetism and ferroelectricity have attracted renewed attention, due to the interesting physics involved as well as relevant potential applications in spintronics. A fairly strong coupling amongst ferroelectric and magnetic order parameters may occur as a result of exchange striction effects in magnetic structures lacking an inversion center. Below the magnetic ordering temperature, slight atomic displacements take place and strengthen (weaken) the satisfied (frustrated) interactions, breaking the inversion symmetry of the structure and leading to ferroelectricity. In this work, synchrotron x-ray diffraction measurements were performed on single crystalline and powder samples of BiMn$_2$O$_5$. A linear temperature dependence of the unit cell volume was found between TN=38 K and 100 K, suggesting that a low-energy lattice excitation may be responsible for the lattice expansion in this temperature range. Between T* ~65 K and TN, all lattice parameters showed incipient magnetoelastic effects, due to short-range spin correlations. An anisotropic strain along the a-direction was also observed below T*. Below TN, a relatively large contraction of the a-parameter following the square of the average sublattice magnetization of Mn was found, indicating that a second-order spin Hamiltonian accounts for the magnetic interactions along this direction. Polycrystalline samples grown by distinct routes and with nearly homogeneous crystal structure above TN presented structural phase coexistence below TN, indicating a close competition amongst distinct magnetostructural states in this compound.

Keywords: BiMn$_2$O$_5$, multiferroics, high-resolution x-ray powder diffraction

P11.12.62

A strategy to prepare multiferroic materials

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Manganese doped bismuth titanate is a potential multiferroic material, displaying both ferroelectricity and ferromagnetism. This is because of the layered nature of the Aurivillius structure which involves the stacking of octahedral perovskite blocks in between layers of bismuth oxide. An n=3 Aurivillius structure, with 3 layers of octahedral units in the perovskite block, are of special interest to solid state chemists. This is because the n=3 arrangement, provides simultaneously, a locally symmetric environment for the B-cations in the middle octahedral layer of the perovskite block and also a structurally distorted environment for the B-cations in the top and bottom octahedral layers of the perovskite block. The stability in maintaining this structural distortion is due to the 6s2 lone pair of electrons from the bismuth in the bismuth oxide layer. This unique structure can accommodate the usually conflicting requirements of ferroelectric and ferromagnetic properties to coexist. The objective would be to incorporate a layer of magnetic manganese cations within the middle octahedral layer, which benefits from the symmetrical environment, and integrate titanium into the top and bottom octahedral layers. This would introduce ferromagnetic properties to bismuth titanate, which is already a well-known ferroelectric material. Synchrotron X-ray diffraction has already been used to determine the structure of some of these compounds and together with magnetic property measurements, it is a step forward in uncovering the relationship between the observed ferroelectric and ferromagnetic properties of these compounds and their atomic structure.

Keywords: materials structure and characterisation, X-ray

powder diffraction, structure-properties relationship
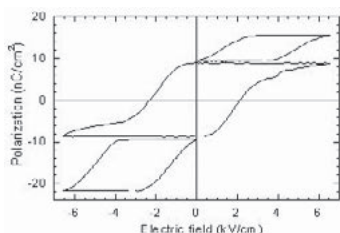
P11.12.63

Discovery of polarization flop and ferrielectric character of multiferroic RMn₂O₅

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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

P11.12.64

Structure and magnetic property of one-dim. chain complex:M^{II}(μ-bpt)(μ-COOC₅H₄N)].H₂O (M=Mn, Fe)

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The one dimensional chain complex, $M^{II}(\mu\text{-bpt})(\mu\text{-COOC}_5H_4N)$]. H_2O (M=Mn, Fe), with the metal centers connected each other with bpt and isonicotinic acid forms an infinite chain along a screw axis 4_1. 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 $I\ 4_1/a$ 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, $[FeN_4O_2]$.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

P11.12.65

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

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Cordierite ($Mg_2Al_4Si_5O_{18}$) 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 Qf 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 $Si_4Al_2O_{18}$ 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.
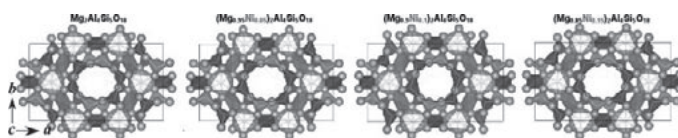

Fig. 1 Structural change on cordierite substituted Ni for Mg.

Keywords: microwave materials, indiarite, order-disorder structure

P11.12.66

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