diffuse scattering or phonon scattering can lead to large effects in the electron diffraction pattern especially near second order phase transition where phonon softening occurs. Additionally, elastic diffuse scattering comes from structural deviations from a periodic lattice [1]. These structural deviations can be defects, partial ordering of otherwise disordered structure or structural fluctuations. By studying diffuse scattering we can obtain information about the crystal imperfections and dynamics which can not be obtained from other characterization methods.
The goal of this study is to characterize, through diffuse scattering in electron diffraction, the structure of defects in the epitaxial layers of perovskite structure and more specifically its influence on the dynamic of the lattice (lattice vibrations, structural fluctuations and continuous phase transition due to phonon softening) [3]. These properties have to be linked with the anomaly of the ferroelectric properties of such thin films. Different strain states can be probed by changing the substrate material or introducing different buffer layers.
The results of STO films deposited on different substrate show different behavior. On STO substrate, at 135K, the superstructure spots in the thin film, have already the same FWHM than the fundamental reflections, indicating a complete phase transition. This shift toward higher transition temperature in thin STO films has already been observed [4]. On LaAlO3 (LAO) substrate, fine peaks appear near 140 K in the diffraction pattern of the film revealing a strain induced phase transition.

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Keywords: thin ferroelectric films; electron diffraction; phase transition

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Magnetic and Dielectric Properties of Fe based Langasites. Pierre Bordet[a], Karol Marty[a], Virginie Simonet[a], Mickael Loire[a], Eric Ressouche[b], Rafik Ballou[a], Celine Darie[a], Jakob Kljun[a], Olivier Isnard[a], Bartosz Zawilski[a], Pascal Lejay[a], Charles Simon[c]. [a]*Institut NEEL, CNRS & UJF, Grenoble, France.* [b]*INAC, SPSMS/MDN, CEA, Grenoble, France.* [c]*CRISMAT, CNRS ENSICAEN, Caen, France.*
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We have investigated the magnetic and dielectric properties of the non-centrosymmetric Fe containing langasites of type $A_3BFe_3D_2O_{14}$ with A=Ba, Sr, Ca, B=Ta, Nb, Sb and D=Ge, Si. Using single crystal and powder neutron diffraction, a novel doubly chiral magnetic order was found in these structurally chiral compounds [1], in which the Fe cations form planar triangular lattices of triangle units. The magnetic structure was found to be a helical spin arrangement propagating along the c axis of equal moments lying in the (a,b) plane at 120°from each other within each triangle. This 120°arrangement results from the usual compromise of frustrated Heisenberg spins on a triangle-based lattice. For all the investigated compounds, the magnetic ordering was found remarkably similar, with Tc ~ 25K and a propagation vector τ~ 1/7, except for those having the B site occupied by Sb^{5+}, for which Tc ~ 35K and τ was closer to 1/5. Unpolarized neutron scattering on a single crystal associated with spherical neutron polarimetry proved that a single triangular chirality together with a single helicity was stabilized in a crystallographically enantiopure crystal. A mean-field analysis allowed us to show that the magnetic and structural chiralities are related though a twist in the plane to plane super-superexchange paths. The langasite structure is non-centrosymmetric P321 and a further lowering of symmetry is achieved in the magnetic phase leaving an overall polar structure for which the appearance of a spontaneous electric polarization is allowed. High resolution synchrotron powder diffraction suggests that the magnetic phase transition could be associated to a structural one. Dielectric measurements reveal the presence of magneto-electric coupling through an anomaly at the Néel temperature in the thermal variation of the dielectric permittivity and its quadratic dependence with the magnetic field. The Fe-langasite could then be a new example enlarging the class of magnetoelectric/ multiferroic triangle-based antiferromagnets

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Keywords: magnetic frustration; dielectric properties; neutron diffraction

FA2-MS05-P10

Ferroelectric Ordering of $Cd_2Nb_2O_7$. Thomas Malcherek. *Mineralogie, Universität Hamburg, Germany.*
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The pyrochlore $Cd_2Nb_2O_7$ (CNO) exhibits unusual ferroelectric properties. Similarity to relaxor materials is indicated by a frequency dependence of the dielectric function over a limited temperature range below 200K. Contrary to standard relaxor material, the formation of polar nanoclusters associated with this behaviour has to be explained in the absence of chemical mixing. Heat capacity anomalies have been observed immediately below 204K, at 85K and at 46K [1]. The exact crystal structure of the corresponding ferroelectric low temperature phases has remained largely undetermined because of their strongly pseudo-cubic nature. Recently the low temperature structure of CNO has been explored by all electron ab-initio calculations in the framework of density functional theory [2]. According to this study, CNO distorts to monoclinic symmetry (space group Cc) at low temperatures via an intermediate orthorhombic phase (space group Ima2). The calculated monoclinic low temperature structure is

characterized by an ordered arrangement of short and long Nb-O-bonds.
In order to verify the results of the computational modeling, single crystal X-ray diffraction measurements have been carried out using synchroton radiation at Hasylab beamline F1. The diffraction data between 200K and 98K are refined on the basis of the calculated Ima2-structure. The ferroelectric order parameter as a function of temperature is obtained and the contributions of various distortional modes are assessed.
While the ab-initio structure calculations imply a purely displacive mechanism of the ferroelectric phase transitions in CNO, anisotropic diffuse scattering intensity that is observed in the X-ray diffraction data indicates local deviations from cubic symmetry in the paraelectric phase. The deviations correlate along <110>, giving rise to sheets of diffuse scattering normal to these directions [3]. In order to investigate the possible order-disorder contributions to the ferroelectric phase transitions, Monte Carlo simulations of a modified 12-state Potts-model on a pyrochlore lattice have been conducted. The equilibrated spin configurations of the model serve to generate supercells of CNO with local Nb-offsets from the center of their coordination polyhedra. The calculated diffraction image based on these supercells reproduces the measured diffuse scattering data qualitatively correct.

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Keywords: ferroelectrics; diffuse scattering; pyrochlore

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Crystal Structure Analysis of Some Metallic Pyrochlores. Yoshitaka Matsushita[a], Kenya Ohgushi[b], Yoshio Katsuya[c], Masahiko Tanaka[a]. [a]*NIMS-Spring8,NIMS, Japan.* [b]*ISSP ,the University of Tokyo, Japan.* [c]*SPring-8 Service Co., Japan.*
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Recent years, the pyrochlore-type compounds ($A_2B_2X_7$ or $A_2B_2X_6$) are very interesting in the field of solid-state physics. For example, $Cd_2Re_2O_7$ [1] and AOs_2O_6 (A = K, Rb, Cs) [2] show superconducting properties and $Cd_2Nb_2O_7$ shows ferroelectric. Most of the properties may be strongly correlated with the structure. The pyrochlore structure has infinite three-dimensional substructure of B-X octahedrons. If we pointed out only B element, the B element forms infinite three-dimensional subunit of B…B tetrahedrons so called as pyrochlore lattice in physics field. This pyrochlore lattice is an origin of strong geometrical frustration effect, and the effect may give a driving force to generate the specific properties such as superconductivity, GMR ($Tl_2Mn_2O_7$) [3], and M-I transition ($Cd_2Os_2O_7$) [4]. On the other hand, as a result of recent study, under low temperature many of pyrochlore-type compounds clearly showed the consecutive structural phase transition with breaking inversion symmetry like the perovskite-type ferroelectric compounds, and the origin of ferroelectrics of the pyrochlore compounds is still unclear. In this study, we are focused on lead-heavy transition metal pyrochores ($Pb_2Ru_2O_7$ and $Pb_2Ir_2O_7$) which have show metallic behavior, and their structural details are also unknown. Therefore, we report the crystal structural details of the compounds ($Pb_2Ru_2O_7$ and $Pb_2Ir_2O_7$). The samples are successfully synthesized by a solid-state reaction. Intensities are measured by powder-diffraction method using high-resolution synchrotron radiation (Spring-8, Japan) at room temperature. Crystal structures are refined by Rietveld method with RIETAN-FP. Both of compounds show the acentric pyrochlore structure with F-43m. The crystallographic details will be presented.

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Keywords: crystal structure and prperties; powder structure determination; synchrotron X-ray diffraction

FA2-MS05-P12

Neutron Diffraction Studies of New Magnetoelectric Perovskites. R. Tellgren[b], S.A. Ivanov[a,b], P. Nordblad[c], C. Ritter[d]. [a]*Dept of Inorganic Materials, Karpov' Institute of Physical Chemistry, Moscow, Russia.* [b]*Dept of Materials Chemistry, The Angstrom Laboratory, Uppsala University, Sweden.* [c]*Dept of Engineering Sciences, Uppsala University, Sweden.* [d]*Institut Laue-Langevin, Grenoble Cedex, France.*
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Magnetoelectrics are materials that are both ferroelectric and ferromagnetic in the same phase. These compounds have potential applications in a whole range of new functional materials. Perovskite oxides containing Pb and Bi cations are particularly promising candidates. Current neutron powder diffraction studies at ILL were focused exclusively on some new and less well studied, but potentially interesting magnetoelectric perovskites.
Pure powder samples were prepared by ceramic technology. X-ray analysis indicated that the compounds have a perovskite-related structure. Magnetic and dielectric measurements were made between 1.5-700 K in order to obtain information about the coexistence range of magnetic and ferroelectric properties. Detailed neutron powder diffraction (NPD) investigations were performed in the temperature range 10-700 K using the D1A diffractometer (ILL, Grenoble, France). NPD powder patterns were registered in the two-theta range 10-160° using λ=1.91 A. The Rietveld method was used for the refinement of the nuclear and magnetic structures.