MS35-04 **Observation of low-symmetry phase in $Na_{0.5}Bi_{0.5}TiO_3$ by optical birefringence microscopy.** Semën Gorfman,[a] Michael Glazer,[c] Pam Thomas[b]
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$Na_{0.5}Bi_{0.5}TiO_3$ (NBT) is a perovskite-based ferroelectric that is currently attracting considerable interest as a potential lead-free piezoelectric material. NBT is unusual in showing two temperature induced phase transformations (see for example [1]), phase coexistence, hierarchical domain systems, strong and anisotropic diffuse scattering, and an ability to form a morphotropic phase boundary (MPB) in solid solutions with other perovskite-based structures. This rich combination of properties means that NBT is not only potential replacement for lead-based piezoelectric materials but also an extremely interesting model system for fundamental crystallography / physics of perovskites and can be studied on its own right. There is a significant amount of X-ray, neutron diffraction and electron microscopy already published and yet considerable disagreement remains concerning the crystal structure and nature of the NBT phases. The aim of this work was to obtain the most precise up to date information about symmetry of a single ferroelectric domain of NBT and reinforce investigation of its temperature dependence. Determination of a true symmetry (crystal class) is mandatory as symmetry plays important role in physical properties of a single domain and a type of a ferroelectric (ferroelastic) domain patterning. To resolve the present controversies about the symmetry of NBT we have undertaken high-resolution reciprocal space mapping of selected Bragg peaks allowing observing fine Bragg peak splitting due to different twin domains [3]. The analysis of separation the beams diffracted by different ferroelastic twin domains suggested that the symmetry of a room temperature NBT must be monoclinic and not rhombohedral as it was commonly accepted before. Above high-resolution X-ray diffraction studies of NBT were complemented by multi-temperature optical birefringence microscopy [2] that is also a sensitive tool to investigate symmetry of a single domain and type of domain pattern. We used the METRIPOL – birefringence microscopy system, equipped with rotatable polarizer, a circular polaring analzer and a high-resolution CCD camera [4]. The collected intensity of light passed through the crystal were converted into the false-colour maps of the magnitude of birefringence and orientation of optical indicatrix, wich is the direct probe of a macroscopic symmetry. The birefringence studies confirmed that the symmetry of NBT is lower than rhombohedral below 300°C and tetragonal above 300°C. The most interesting result of this work is that the in some case the rotation of a polar direction within a monoclinic plane were directly observed. The peculiar temperature induced transformations of symmetry and domain patterns as visible by birefringence microscopy will be discussed in the talk.

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Keywords: ferroelectric crystals; symmetry; birefringence

MS35-05 **Symmetry adapted analysis of the magnetic and structural phase diagram of $Bi_{1-x}Y_xCrO_3$.** Claire V. Colin, Pierre Bordet, Céline Goujon, and Céline Darie, *Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France*
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Bismuth based perovskite compounds $BiMO_3$ (M=transition metal) have recently attracted a lot of attention due to the possibility of intrinsic multiferroism. One of the least investigated compounds of the series is $BiCrO_3$, probably because it can only be synthesized under high pressure. Understanding multiferroism in a complex material such as $BiCrO_3$ cannot be envisaged without establishing the close relationship between structural and magnetic properties. To do so we have applied the following approach: (i) the monoclinic structural distortion of $BiCrO_3$ was tuned by isovalent substitution of Bi^{3+} by Y^{3+} which does not possess a stereoactive electronic lone pair; (ii) the magnetic structures and active distortion modes have been determined by refinement of neutron and x-ray powder diffraction data using the symmetry mode analysis concept. This method allowed us hierarchizing distortion modes and identifying those which stabilize the various distorted structures with respect to the cubic perovskite one. Since the structural distortions are related to the magnetic super-exchange through the control of orbital overlaps, this procedure is well suited to reveal the links between structure and magnetic ordering in this quite complex system.

$Bi_{1-x}Y_xCrO_3$ compounds were synthesized under high pressure and high temperature. The magnetic and structural phase diagrams were established by means of magnetization measurements, x-ray and Neutron Powder Diffraction (ILL-D1B and LLB-G4.1). We found that the monoclinic distorted structure is replaced by the orthoferrite-type orthorhombic structure for $x \geq 0.05$. NPD experiments revealed that all compounds display G-type antiferromagnetic structures. However, the direction of the spins changes with Y^{3+} content: spins are aligned along the b-axis (Γ_7 magnetic representation) for yttrium-poor compounds and along the c-axis (Γ_5 magnetic representation) for yttrium-rich compounds. Symmetry adapted analysis indicated the primary importance of the LD3 distortion mode for the stabilization of the monoclinic structure and its antiferroelectric arrangement. The interplay between crystal distortion modes and magnetic properties will be discussed.

Keywords: structural and magnetic phase transitions; structure-magnetism relationships; group theory