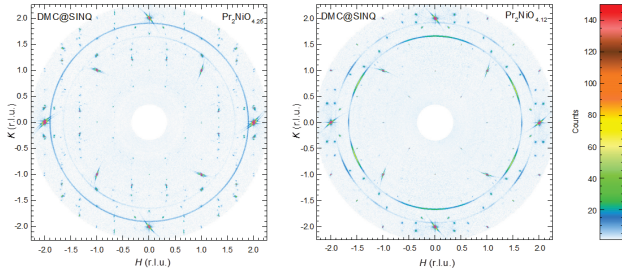

Figure 1. HK0 maps of Pr_2NiO_{4+d} single crystals with d=0.25 (left) and .12 (right) at T=100K collected at DMC@SINQ (a=b~3.8Å, c~12.3Å). Additional peaks originate from the oxygen superstructure which in the case of d=0.12 partly vanish at room temperature.

Keywords: oxygen diffusion, perovskites, functional structures, sustainable materials

MS16-P7 On the tetragonal phase of sodium bismuth titanate, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT)

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Sodium bismuth titanate, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), has attracted attention as a potential component of lead-free piezoelectrics with the ultimate aim of replacing the industrial standard material lead zirconate titanate (PZT). At room temperature the crystal structure is monoclinic pseudo-rhombohedral on average (space group Cc or disordered *R3c*). Above ~ 573K on heating, the structure is tetragonal, solved by Jones & Thomas [1] in *P4bm*. Above ~ 833K it becomes cubic (*Pm-3m*).

NBT can be combined with $BaTiO_3$ (BT) amongst other useful perovskites, to make the solid-solution NBT_{1-x}-BT_x (NBT-BT). BT is tetragonal (*P4mm*) at room temperature and its solid-solution with NBT can be described by R3c up to x ~ 0.06. At x = 0.06, it was thought that the structure changed abruptly from rhombohedral to tetragonal in an analogous fashion to the so-called morphotropic phase boundary in PZT. However, subsequent works showed that the transition is rather more gradual and that a fully tetragonal polar structure described by *P4mm* is not established until x > 0.1-0.15 [2]. Ma & Tan reported that the transition between the ferroelectric rhombohedral and tetragonal phases in NBT-BT takes place via a pseudo-cubic weakly polar region of composition space assigned as *P4bm*. This phase can be prompted into a more strongly polar phase by application of an electric field [3], referred to as an E-field induced phase transition if the new state persists after the E-field is removed. The understanding of this E-field induced behaviour and the favourable physical properties that accompany it are predicated on understanding the structure and nature of the *P4bm* phase itself.

New detailed parametric structural data for NBT are presented in the temperature range from 573-943K. The tetragonal phase region is bounded by metrically cubic phases at both high and low temperatures, with the high temperature phase being the cubic aristotype. The tetragonal strain is maximum at 670(±5)K. New structural refinements in key regions of the temperature phase diagram are presented and correlated with physical property data, particularly optical birefringence measurements from single crystals [4] and results of pair distribution function (PDF) analysis.

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