MS13-2-10 Following the path of temperature-induced phase transitions in $Pb(Mg_{1/3}Nb_{2/3})$ – $PbTiO_3$ ferroelectric crystals
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Abstract
(1-x) Pb(Mn1/3Nb2/3)O3 - x PbTiO3 (PMN-PT) is a functional ferroelectric material that has many technologically important applications as sonars for underwater communications, actuators and ultrasonic transducers [1]. The functionality of PMN-PT is underpinned by the flexibility of its perovskite-based structure and the ability to form complex domain microstructures through the various structural phase transitions. These transitions (between para- and ferroelectric as well as between different ferroelectric phases) have been in focus of much research [2] since the discovery of this material. The structure and symmetry of PMN-PT depends on its composition, x, and the temperature, T: it includes cubic, tetragonal, rhombohedral and two types of monoclinic phases. Because the delineation between these phases remains the major experimental challenge, certain areas of the x-T phase diagram are still rather vague. In addition, most of the existing structural studies of PMN-PT are performed with relatively coarse (> 15 K) temperature steps.
The aim of the work is to advance the understanding of the phase transitions in PMN-29PT and PMN-35PT crystals by tracing their cubic-tetragonal and tetragonal-to-monoclinic phase transitions using high-resolution single crystal X-ray diffraction. We collected a series of 3D reciprocal space volumes (RSV) which represent diffraction intensity distribution around certain families of Bragg peaks. Such Bragg peaks split into several components due to the presence of ferroelastic domains. The analysis of such splittings offers a powerful tool for elucidation of single-domain symmetry, and twin relationship between the domains [3]. We used a custom-built four-circle X-ray diffractometer, equipped with the microfocus X-ray source, double-crystal monochromator, Eulerian cradle, PILATUS 1M pixel area detector and fine-temperature control sample environment cell [4]. We measured RSVs around selected Bragg peaks with very fine (~0.1 K) temperature steps, both on heating and cooling. From their analysis we could follow the phase transitions path over between the room temperature and the transition to the cubic phase. We determined the phase transition temperatures on heating and cooling. By doing so, we characterised the order of the transition and checked the associate fine details. In addition, we were able to characterise the details of domain patterns occurring during each phase transition.
In the figure attached (Figure 1), one can see the change of the RSVs of PMN-29PT upon fine temperature steps. Noticeably, the shape of the peak differs as the phase transitions take place ((a) and (e) monoclinic phase; (b) and (d) tetragonal phase; (c) cubic phase).

References
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Figure 1