MS32-1-1 Identification of a coherent twin relationship in functional perovskites from high-resolution reciprocal-space maps
#MS32-1-1

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Abstract
Twinning is a common crystallographic phenomenon, related to the formation and coexistence of several orientation variants of the same crystal structure. It may occur during symmetry-lowering phase transitions or crystal growth itself. Once formed, twin domains play an important role in defining physical properties of functional materials: for example, they underpin the giant piezoelectric effect in ferroelectrics, superelasticity in ferroelastics and the shape-memory effect in martensitic alloys. Unfortunately, there is still a lack of experimental methods for the characterization of twin domain patterns. Although single crystal X-ray diffraction could fill this methodological gap, its implementation for the case of diffraction from multi-domain crystal is far from trivial especially for the case of the so-called pseudomerohedral twinning. Specifically, it is hard to assign various components of split Bragg peaks to the particular set of domains.
Here we propose a theoretical framework and an algorithm for the recognition of ferroelastic domains and the identification of the coherent twin relationship using high-resolution reciprocal space mapping of X-ray diffraction intensity around split Bragg peaks. We adapt the geometrical theory of twinned ferroelastic crystals [1] for the analysis of the X-ray diffraction patterns. We derive the necessary equations and outline an algorithm for calculation of the separation between the Bragg peaks, diffracted from possible coherent twin domains, connected to one another via mismatch-free interface. We demonstrate that such separation is always perpendicular to the planar interface between mechanically matched domains.
As examples, we present the analysis of the separation between the peaks diffracted from tetragonal and rhombohedral domains in the high-resolution reciprocal space maps of $BaTiO_3$ and $PbZr_{1-x}Ti_xO_3$ crystals of functional ferroelectric perovskites. We collected three-dimensional reciprocal space maps at the custom-built home-laboratory four-circle X-ray diffractometer [2], equipped with large (PILATUS 1M) pixel area detector. The example of such reciprocal space map of diffraction intensity distribution around 102 Bragg peak of $BaTiO_3$ is presented in the Figure 1. The analysis (see [3] for full details) results in the assignment of the present peaks to specific sets of ferroelastic domains as well as establishing the orientation of domain walls between them.
The method can be used to analyse the response of multi-domain patterns to external perturbations such as electric field, change of a temperature or pressure.

References
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Figure 1