Recognition of ferroelastic domains in high-resolution X-ray diffraction patterns

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Twinning is a common crystallographic phenomenon, which occurs in some crystals during a symmetry-lowering phase transition. Twin domains and domain walls play important role for physical properties, e.g. underpin giant piezoelectric effect, superelasticity and shape-memory effect. The formation of ferroelastics (=strain) twin domains is common in broad class of materials including perovskite oxides and martensitic alloys. Understanding the properties and the geometry of ferroelastic domain patterns is challenging but necessary. There is still a lack of experimental methods for imaging and characterization of twin domain patterns.

Here, we propose a theoretical framework and an algorithm for the recognition of ferroelastic domains using high-resolution X-ray diffraction / reciprocal space mapping (Figure 1 shows an example of such reciprocal space around 102 reflection of $BaTiO_3$). We adapt the existing geometrical theory of twinned ferroelastic crystals [1] for the analysis of X-ray diffraction patterns. We derive the necessary equations and outline an algorithm for the 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 arises along the direction, perpendicular to the planar interface between mechanically matched domains.

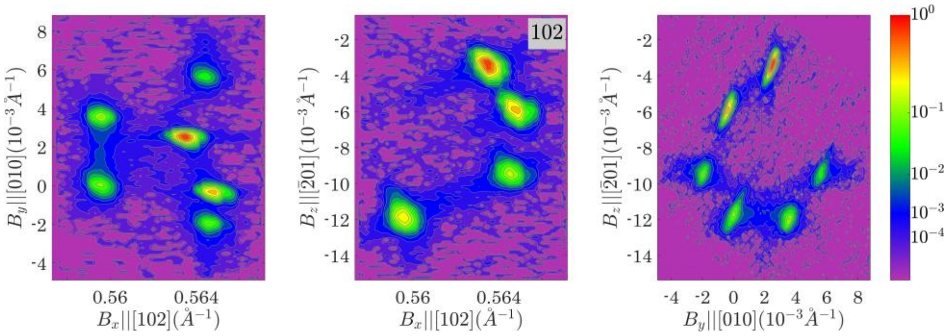

Figure 1.

High-resolution reciprocal space map collected from multi-domain tetragonal $BaTiO_3$ crystal.

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. Reciprocal space maps were collected at the custom-built four-circle X-ray diffractometer, equipped with PILATUS1M pixel area detector [2]. The demonstrated method can be used to analyze the response of multi-domain patterns to external perturbations such as electric field, change of a temperature or pressure.

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