Recognition of ferroelastic domain patterns using high-resolution single crystal X-ray diffraction: potential for DFXM

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Ferroelectric / ferroelastic / ferroic domains are the volumes of a material where polarization / strain / any other order parameter are uniform. Domain patterns appear because of a structural phase transition between phases of different symmetries. They play important role for the materials properties, e.g. domain-wall motion may contribute to the enhancement of piezoelectric effect and dielectric permittivity. Although the knowledge of domain patterns geometry is crucial for the ability to characterize, predict and even tailor the properties, only a handful of penetrating and non-destructive experimental techniques are available for the characterization of ferroic domain patterns in the bulk of a material. X-ray diffraction and dark-field X-ray microscopy are certainly capable of filling this gap.

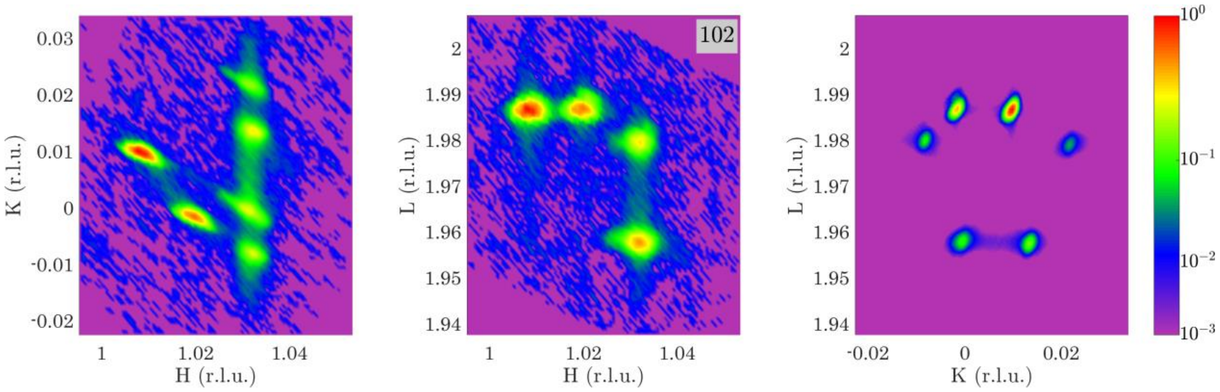

Figure 1: Three-dimensional reconstruction of X-ray diffraction intensity distribution in the reciprocal space 102 family of Bragg peaks of $BaTiO_3$ single crystal

Geometry of ferroelastic domain patterns is governed by the laws of mechanical compatibilities of domains, formulated in [1]. The goal of this work is to extend this formalism of mechanical compatibilities to enable effective analysis of diffraction patterns from ferroelastic domains such as the one from $BaTiO_3$ shown in the Figure 1. Specifically we obtain relevant analytical expressions for the reciprocal space separation between the peaks diffracted from different domains. Additionally we develop computer algorithm, which recognizes contribution of domains (orientation of domain walls) in three-dimensional reciprocal space maps obtained from multidomain ferroelastic crystals. While the developed method assumes the availability of the reciprocal space information alone, it may also greatly assist in the interpretation of the X-ray microscopy data.

We will demonstrate the application of the developed method for the recognition of ferroelastic domains in the reciprocal space maps of tetragonal $BaTiO_3$ crystal. Additionally we will discuss the potential of method in assisting the analysis of the dark field X-ray microscopy data.

[1] J. Fousek, V. Vanocek., Journal of Applied Physics **40**(135), 135-142, (1969).