MS42-05 | Inspecting Piezoelectricity in $PbZr_{1-x}Ti_xO_3$ Single Crystals with Ferroelastic Domains

Gorfman, Semën (Tel Aviv University, Tel Aviv, ISR); Choe, Hyeokmin (Tel Aviv University, Tel Aviv, ISR); Nan, Zhang (Electronic Materials Research Laboratory, Xi'an, CHN); Chernyshov, Dmitry (SNBL at the ESRF, Grenoble, FRA); Ye, Zuo-Guang (Department of Chemistry and 4D Lab, Simon Fraser University, Vancouver, CAN)

Piezoelectricity is the ability of some materials to get electrically polarized under mechanical stress and mechanically deformed under electric field. Despite increasingly high demand and expanding realm of application, the choice of practically explored piezoelectrics is limited to quartz (a-SiO_2) crystals, $PbZr_{1-x}Ti_xO_3$ (PZT) ferroelectric ceramics and $PbMg_{2/3}Nb_{1/3}O_3$ - $PbTiO_3$ (PMN-PT) relaxor-ferroelectric crystals. Piezoelectricity is well studied phenomena, however, some aspects like the role of ferroelectric / ferroelastic domains) remains poorly understood. Therefore, the design of new functional piezoelectrics – e.g. lead-free alternatives to PZT remains complicated.

Here we develop X-ray diffraction-based technique and data-analysis algorithm for separation of "domain-related" and "intrinsic" response of ferroelectric / ferroelastic domains in PZT single crystals to external electric field. We measured three-dimensional high-resolution reciprocal space maps around selected families of split Bragg peak, representing diffraction from differently oriented ferroelastic twin domains. The crystal was loaded into specially designed sample environment cell [1], while external electric field was synchronized with PILATUS2M detector using microcontroller-based data-acquisition system [2]. We developed the algorithm for assignment of different components of each family to individual domain variants with known direction of spontaneous polarization relative to applied electric field. Using this algorithm, we are able to track the change of lattice constants and domain volume fraction of each domains.

[1] T. Vergentev et al. J. Appl. Crystallogr. **49**, 1501 (2016).
[2] H. Choe et al. J. Appl. Crystallogr. **50**, 975 (2017).