Exploring twinning laws in functional ferroic through high-resolution X-ray diffraction

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Abstract:

Formation of twin domains is prevalent in ferroelectric, ferroelastic, and martensitic materials due to symmetry-lowering phase transitions. Besides its intrinsic crystallographic appeal, twin domains may become functional when housing specific order parameters like polarization, magnetization, or strain. Particularly when some order parameters coexist, domains may be switched by external fields, enabling, for example, giant electromechanical activity. Despite significant interest, functional twinning remains poorly understood because current experimental investigation techniques lack the ability to provide a full picture. For example, piezo-response force microscopy and optical microscopy are limited to surfaces or thin, transparent samples. Incorporating non-destructive X-ray diffraction technique for this purpose could significantly enhance this area.

The goal of our work is to introduce high-resolution single-crystal X-ray diffraction for the characterization of twinning in functional ferroelectric materials. We use the previously existing concept of permissible domain walls (PDW), where the PDW stands for a domain wall that provides a connection between two domains without any lattice mismatch. We extend the mathematical framework of PDW and add all the features necessary to enable it for the analysis of three-dimensional reciprocal space maps. Our reshaped theory enables modeling the separation of Bragg peaks diffracted from matched domains. We present an algorithm and computer program for peak assignment to specific domains, illustrated using tetragonal, rhombohedral, and monoclinic ferroelectrics. These findings advance understanding of domain formation during phase transitions and domain-wall motion-driven properties.

Shot Biography

Dr. Gorfman, an Associate Professor at TAU's MSE Department, received his MSc in Physics from Chelyabinsk State University, Russia, and a PhD in Physics from the University of Siegen, Germany. Prior to joining TAU in 2017, he was a postdoc at the University of Warwick, UK (2008–2011), and a lecturer at the Universities of Siegen and Freiburg, Germany (2011–2017). His research focuses on fundamental and X-ray crystallography, crystal properties, piezoelectrics, ferroelectrics, and in-situ X-ray diffraction studies. Dr. Gorfman conducts his research primarily at synchrotron radiation and neutron scattering facilities, with notable contributions in investigating ferroelectric perovskite oxides' fine structure, symmetry, and functionality.