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Short-range atomic ordering in PbZrxTi1-xO3 single crystal revealed by diffuse scattering and 3D-△PDF modeling

Content

The PbZrxTi1-xO3 (PZT) solid solution is one of the most widely applied ferroelectric materials due to its excellent electromechanical properties. However, despite the extensive studies in the past half century, the physical origin of its properties is still not fully understood, which is mainly caused by the complexity of its crystal structure, especially in the local atomic scale [1]. By electron diffraction with ferroelectric PZT [2], it was found that the diffuse scattering (DS) intensity form {111} planes, while a complete local-structural model of such DS pattern still lacks.

In this study, we performed x-ray DS experiments with PZT single crystals (x~0.4) with average rhombohedral symmetry at room temperature, and reconstructed the three-dimensional distribution of the DS intensity in full reciprocal space (Fig. 1a). To get quantitative information out of this distribution of DS intensity, we constructed a difference-pair-distribution-function (△PDF) model with short-range correlation of atomistic displacements, and refined this model against the experimental data using the software Yell [3]. The feature of DS intensity was successfully reproduced with the refined model (Fig. 1b). From the model, it is revealed that there exists various types of short-range displacive correlations between neighboring Pb atoms and they may be the result of the impact of surrounding Zr4+ and Ti4+ cations. This study provides a more-complete understanding of the local atomic behavior in ferroelectric crystals with long-range ordered cation displacements.

References:

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[3] Yell : a computer program for diffuse scattering analysis via three-dimensional delta pair distribution function refinement, J. Appl. Crystallogr. 47, 1146 (2014).

Primary author: AN, Zheyi (Xi'an Jiaotong University)

Co-authors: Dr PAŚCIAK, Marek (Institute of Physics of the Czech Academy of Sciences); Prof. SIMONOV, Arkadiy (ETH Zurich); Prof. ZHANG, Nan (Xi'an Jiaotong University)

Presenter: AN, Zheyi (Xi'an Jiaotong University)

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