Oral presentation

Characterization of domain wall mobility in piezoelectric single crystals from high-resolution x-ray diffraction

Nan Zhang[1], Guanjie Zhang[1], Sem Gorfman[2]

[1]Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research, School of Electronic and Information Engineering, Xi'an Jiaotong University, Xi'an, People's Republic of China

[2]SDepartment of Materials Science and Engineering, Tel Aviv University, Tel Aviv, Israel

nzhang1@xjtu.edu.cn

Piezoelectric materials are utilized in various applications, including ultrasonic transducers, sensors, actuators, and frequency generators. The extrinsic contribution from the domain wall motions plays an essential role in the piezoelectric effect. However, the detailed understanding of the domain-wall mechanisms still needs to be improved and expanded, especially for the complex coexistence of multiple domains. The *in situ* high-resolution x-ray diffraction is a powerful technique for probing structural information, especially domain structures, of ferroelectrics under external stimuli [1, 2]. The positions of each Bragg reflection are related to the lattice vectors of each domain and the orientation of the domain walls can be calculated correspondingly.

Here, we uncover the influence of domain volume fraction on domain wall motion in $PbZr_{0.52}Ti_{0.48}O_3$ single crystals throughout the monoclinic to tetragonal phase transition using high-resolution single-crystal synchrotron x-ray diffraction and mechanical compatibility theory. We find that the domain wall orientation strongly influences the three-dimensional diffraction intensity distribution, allowing us to trace the domain wall orientation change with temperature. The evolution of the domain walls proves that the different domain volume fractions lead to diverse evolutionary behaviors of the domain walls. The domain pairs with a large volume fraction form the stable domain wall, while those with a small volume fraction form the susceptible domain wall. Our discovery is a step towards a deeper understanding of domain wall motion and offers a promising method to enhance the piezoelectric effect by controlling the domain structures and domain volume fractions in piezoelectric crystals.

[1] Zhang, N., Gorfman, S., Choe, H., Vergentev, T., Dyadlin, V., Yokota, H., Chernyshov, D., Wang, B., Glazer, A. M., Ren, W. & Ye, Z.-G. (2018). *J. Appl. Cryst.* **51,** 1396.

[2] Gorfman, S. Spirito, D., Zhang, G., Detlefs, C. & Zhang, N. (2022). *Acta Cryst*. *A* **78,** 158.