Interface Orientations in Relaxor Ferroelectrics Measured by Diffuse Scattering

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Relaxor ferroelectric materials are a particular category of ferroelectrics that possess high dielectric constants and large electromechanical constants. This makes them particularly attractive for applications such as ultrasonic transducers and electromechanical actuators. Their specific properties are governed by characteristics including composition, crystallographic phase, and nano- to mesoscale disorder and domain structures. Diffuse X-ray scattering in relaxor ferroelectric crystals provides information on the state of disorder. This can include atomic occupational disorder, as well as nano-scale domain structures that break the long-range symmetry of the system. Here, we use high-energy diffuse X-ray scattering to study the electric field and stress induced transitions in a PIN-PMN-PT crystal when driven from a 2R engineered domain state to a 10 domain state [1]. It's shown that the diffuse streaking associated with the nano-domain structure is removed on driving from the polydomain, 2R, to the monodomain, 1O, state (Figure 1). Analysis of multiple stepwise points along this transition pathway aid in providing mechanistic understanding of electric field and stress induced transformations in relaxor ferroelectrics. These findings will help guide optimal compositional and usages cases for transducer design and fabrication.



Figure 1. Demonstration of the relationship between long-range breaks in symmetry and diffuse scattering streaking as calculated by FFT modelling and the diffuse scattering from the (200) reflection of a PIN-PMN-PT crystal at low- and high-electric field conditions displaying a disappearance of streaking pattern.

[1] Finkel, P., Cain, M. G., Mion, T., Staruch, M., Kolacz, J., Mantri, S., Newkirk, C., Kavetsky, K., Thornton, J., Xia, J., Currie, M., Hase, T., Moser, A., Thompson, P., Lucas, C. A., Fitch, A., Cairney, J. M., Moss, S. D., Nisbet, A. G. A., Daniels, J. E., Lofland, S. E., (2022) *Adv. Mater.* **34**, 2106827.