Quantitative mapping of nanotwin variants and elastic energy in the bulk

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Even most state-of-the-art high-resolution imaging techniques are limited to probing the sample surface. This is a particular drawback for the characterization of twinned materials as the strain state changes from biaxial at the surface to triaxial in the bulk, [1] dramatically influencing the functional properties. One way around this is Dark-field X-Ray Microscopy, which was recently applied to visualize long ranging strain fields in the vicinity of embedded ferroelastic domain walls and grain boundaries in the bulk. [2] The resolution, however, is determined by the optics of the lenses, which prohibits investigations on nano-sized domains common in twinned materials.

Here, we overcome this limitation by using the full reciprocal-space intensity distribution allowing mapping of nanotwin variants highly localized in the bulk (Figure 1). [3] We demonstrate the methodology for a high-performance polycrystalline ferroelectric/ferroelastic $(Ba,Ca)(Zr,Ti)O_3$ model system whose excellent piezoelectric properties originate from domain sizes of 10-100 nm. We corroborate our proposed methodology by simultaneously quantifying the elastic energy *in-situ* under different applied electric fields. For all electric fields, we find that the density of twin variants is coupled to the elastic energy. For example, the density of twin variants inside the grain is 30% smaller compared to the density in the vicinity of the grain boundary, following the trend of the elastic energy. The obtained elasto-morphological correlations are crucial for many twinned materials, ranging from complex oxides to martensitic materials or high entropy alloys.

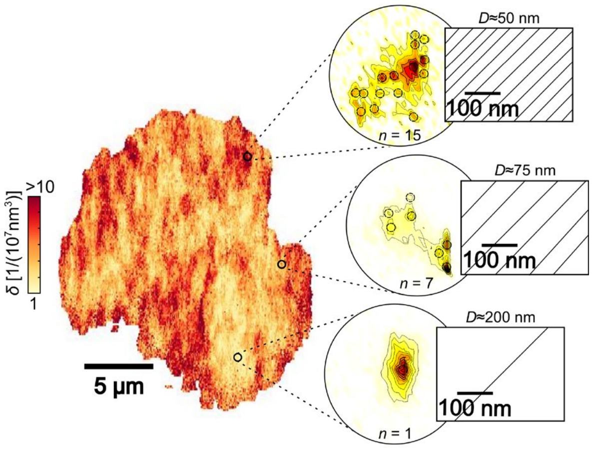

Figure 1: Mapping of the density of twin variants, δ, and their estimated sizes, D, in the bulk of a nano-twinned piezoceramic material. The density of twin variants is displayed spatially resolved for the cross section of a grain. The density of twin variants was obtained by systematically monitoring reciprocal-space intensity distributions from grain subvolumes obtained by Dark-field X-Ray Microscopy.

References
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