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Supporting information for article:

Understanding nanoscale structural distortions in Pb(Zr0.2Ti0.8)O3 by utilizing X-ray nanodiffraction and clustering algorithm analysis

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1. Rocking curve of the PZT sample

The rocking curve of the PZT thin film using laboratory x-ray diffraction Cu Kα source) is shown in Figure S1. The full width at half maximum (FWHM) of the (002) PZT rocking curve is 0.158°, which corresponds to the averaged mosaicity of the as-grown PZT film.

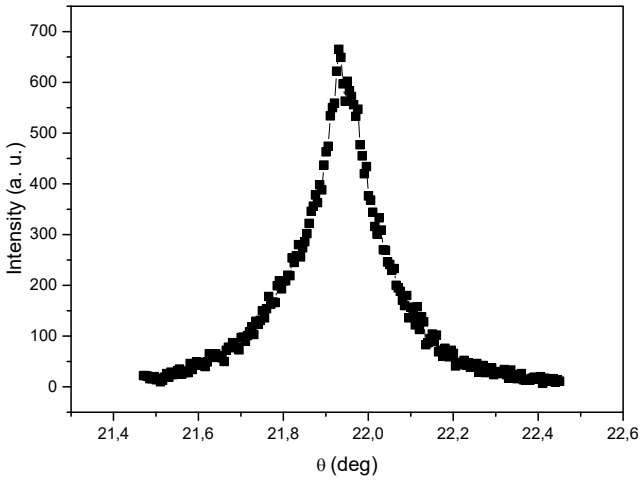

Figure S1: (002) rocking curve for the PZT thin film (FWHM =0.158°)

2. Centroid calculation method for nanodiffraction datasets

In order to quantify local strain variation, centroid calculation within a region of interest (ROI) is typically used to calculate the 2θ-value and obtain lattice parameter for nanodiffraction datasets (Holt *et al.*, 2013; Jo *et al.*, 2011; Rippy *et al.*, 2019). Figure S1(a) shows a thin horizontal ROI usually utilized for calculating centroid position However, it can be easily seen that such a ROI will either miss the intensity maxima or will obscure the signal due to multiple peaks present in the diffraction pattern. Specifically, due to peaks present at both the left and the right side of the annulus, typical centroid calculation will miss the accurate centroid determination due to averaging effects. Figure S1(b) shows a lattice parameter map with such a ROI, and no difference in lattice parameter for up and down domain can be observed, indicating that such an analysis method is insufficient to obtain nanoscale variation of the lattice parameter in mosaic samples. Here we note that the horizontal shift or translation of the entire diffraction pattern overlaid on the annulus on the detector occurs due to mosaicity of the sample (slight tilting of atomic planes) and does not contribute to local strain as discussed by Holt *et al.* (2013). This effect has been accounted in the lattice parameter calculation shown in Figure S1(b) as well as in the main article.

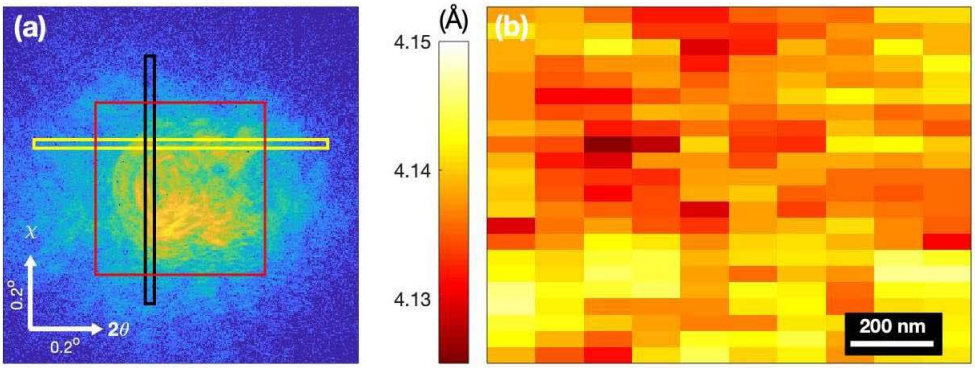

Figure S2: a) Typical ROIs used in previous analysis methods, b) lattice parameter map obtained by calculating centroid of the horizontal ROI. No clear demarcation between up and down domain is observed in the lattice parameter distribution.

3. ROI selected for K-means cluster analysis

Twelve different ROIs were selected as shown in figure S2(a)-(d) that subdivide the diffraction pattern into different regions extending beyond the boundaries of the annulus. These ROIs were selected to cover the diffraction pattern in different ways, so that the new approach is independent of ROI as well as not reliant upon presence of a single peak i.e. in mosaic or phase-separated samples.

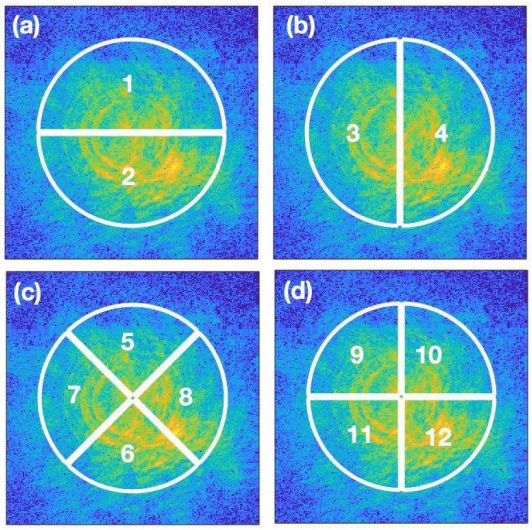

Figure S3: ROIs used in cluster algorithm analysis

References

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