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Mapping Polar Distortions with Nanobeam Electron Diffraction with a Cepstral Approach

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Understanding local polar ordering is key to understanding ferroelectricity in thin film systems, especially for systems with small domains or significant disorder. Scanning nanobeam electron diffraction (NBED) combined with new high speed, pixelated scanning transmission electron microscopy (STEM) detectors make it possible to measure a diffraction pattern (k_x, k_y) at every scan position (x, y). This opens doors to investigate lattice parameters, local fields, polarization directions, and charge densities with relatively low beam dose over large fields of view. However, quantitatively extracting both the magnitude and direction of polarization vectors is still challenging. Here we use a cepstral approach, similar to a 2D pair-correlation function, to measure these local polar displacements that drive ferroelectricity.

The magnitude of the Fourier transform of the logarithm of the NBED pattern generates the power cepstrum (PC) [1], which has sharp peaks at the real-space interatomic distances in a crystal (Figure 1, first and second column). This is similar to a pair-distribution function or Patterson function, but remarkably robust to specimen mistilt and thickness [1]. However, this transform discards information about asymmetry in the diffraction pattern, including those from polar components of the lattice. Here we extend this approach to use the complex value of the Fourier transform (the complex cepstra, CC), recovering the asymmetrical information in the diffraction pattern. In electron diffraction patterns, polar distortions generate an asymmetry in the diffraction pattern, breaking Friedel's law such that the relative intensities of the hkl and $\bar{h}\bar{k}\bar{l}$ spots are no longer the same (see the logarithm of the NBED patterns for some polar materials in Figure 1). To efficiently extract information about the non-centrosymmetric components of the crystal, we use the imaginary component of the Fourier transform (Figure 1, third column). The features of the PC and CC transforms can be directly related to the symmetric and antisymmetric components of the crystal structure, which is shown in the last column of Figure 1, to scale).

In this presentation, we will discuss the application and limits of this technique and map polar distortions across a thin film of $PbTiO_3$ (Figure 2) and in relaxor ferroelectrics.

References:

[1] E. Padgett, M. E. Holtz, P. Cueva, Y.-T. Shao, E. Langenberg, D. G. Schlom, and D. A. Muller, Ultramicroscopy **214**, 112994 (2020).

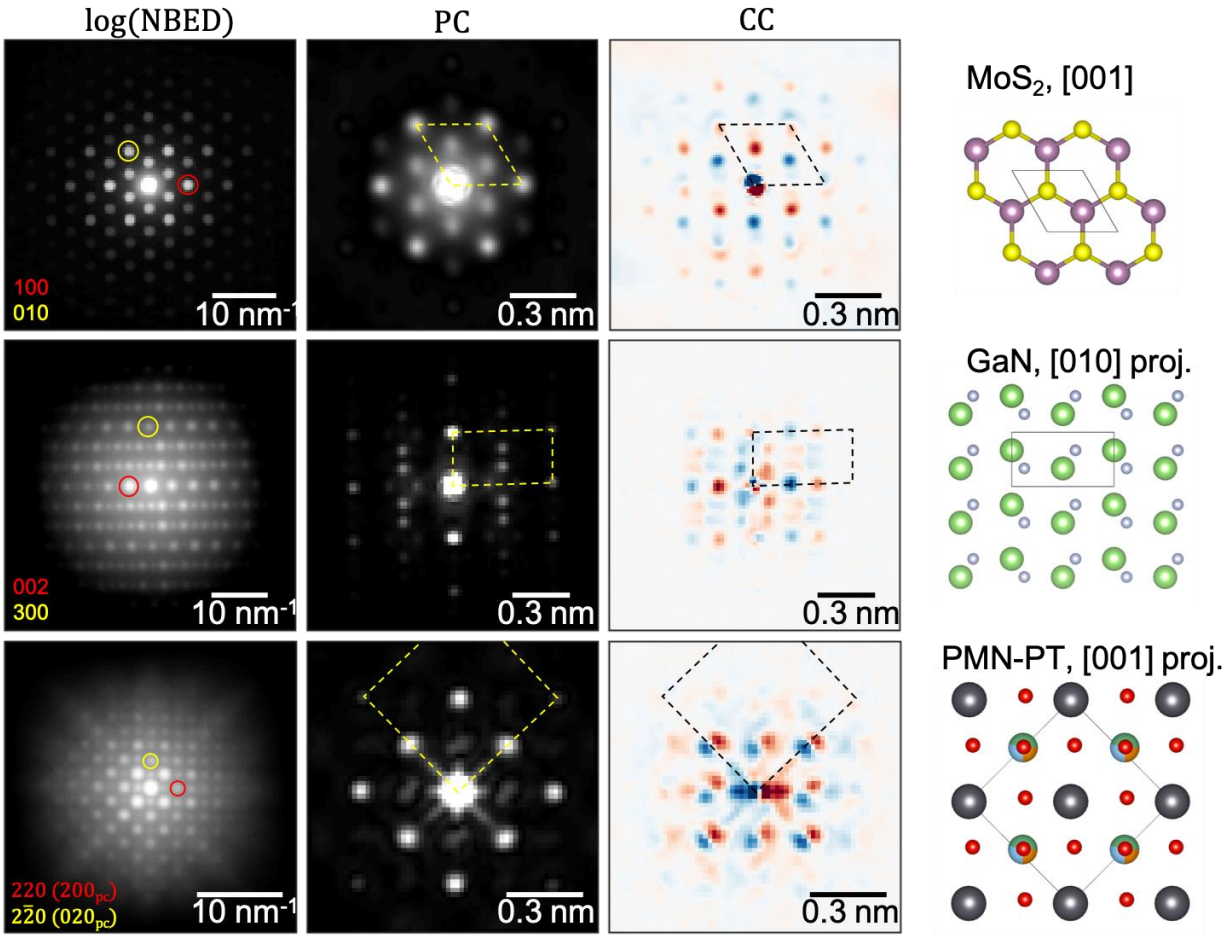

Figure 1. The log(NBED) patterns, PC transforms, and CC transforms for three polar materials. The PC transform has peaks for interatomic spacings. The CC transform is false-colored with red being positive values and blue being negative values. The dipoles in this transform relate directly to the polarity in the crystal.

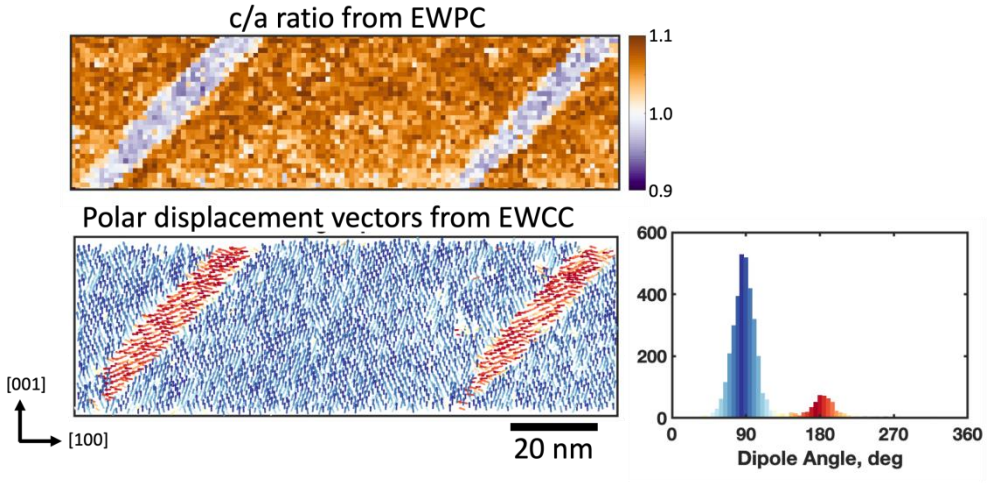

Figure 2. The c/a ratio measured by the PC transform and the polar displacement vectors measured by CC for $PbTiO_3$ thin film. Colors for the displacement vectors are in the histogram.

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