

## Denoising 4D STEM datasets with PCA

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Background incl. aims

4D Scanning Transmission Electron Microscopy (4D STEM) provides crucial insights into materials structures by utilizing Differential Phase Contrast (DPC), ptychography, orientation and strain mapping. However, 4D STEM datasets often suffer from noise, hindering accurate analysis. It would be desired to denoise 4D STEM data by Principal Component Analysis (PCA) as it was successfully applied for EELS and EDX STEM datasets [1]. Additionally, PCA allows for accurate separation of the constituting compounds by clustering in the latent PCA factor space.

Methods

The sample used for this demonstration is organic solar cell blend DRCN5T:PC71BM solvent vapour annealed in chloroform. The 4D STEM dataset was obtained in micro-probe STEM (convergence angle ~1 mrad) with a Titan Themis microscope operating at 300kV. The data was collected using a OneView IS detector operating at frame rate of 400 fps (2.5 ms frame time) and probe current of about 5 pA.

We developed a Python-based PCA routine and integrated it into the temDM in-house developed 'Spectrum Imager' tool. This tool, originally designed for visualizing and denoising EELS and EDX spectrum-images [2], is presently adapted for 4D STEM datasets processing, including re-centring, clipping, viewing with virtual circular/ring apertures et cet. [3].

Results

When scanning the focussed beam across a sample, a shift of the diffraction pattern inevitably occurs, known as the pivot effect. While this effect can be minimized through accurate instrument tuning, it cannot be eliminated completely. We found that even a slight pivot effect dramatically influences PCA results, overriding any structural variations. In the considered example, the pivot shift within the scanned field of view was less than 2 pixels. Nevertheless, the data variation in the PCA factor space predominantly reflected the pivot variation rather than the structural changes in the sample (Fig.2, upper).

The diffraction shift was measured with the sub-pixel precision in each individual diffraction pattern using the centre-of-mass method. It is important to note that simply centring the patterns is not an option as this would preclude any DPC measurements. Instead, we assumed that the pivot shift

changes linearly along both x- and y- directions and calculated this by the least-square fit. The diffraction patterns were then shifted with the cubic-spline interpolation to account for the linear pivot. After the consequent PCA, the principal components clearly revealed the structural changes in the sample (Fig.2, lower).

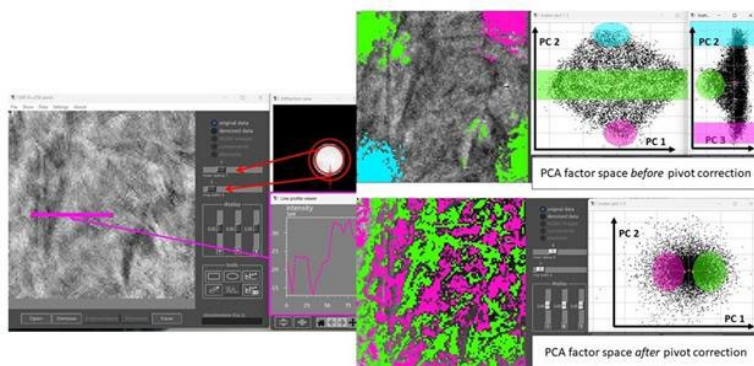
### Conclusion

4D STEM datasets can be successfully denoised by PCA, however it requires precise data pre-processing, particularly addressing the pivot shift. The sub-pixel interpolation is mandatory for the accurate subtraction of the pivot shift.

### Figure caption

Impact of pivot correction on PCA results. The clusters are selected as hypercylinders in the latent PCA factor space. Without correction, instrumental pivot shift dominates in the PCA factor space. After correction, clustering in the factor space clearly reveals the structural compounds.

### Graphic:



### Keywords:

4D STEM, software, PCA, denoising

### Reference:

- [1] M. Watanabe et al. Microsc. Microanal. 11, 5, 2009.
- [2] P. Potapov et al. #0132. Proc. Int. Microscopy Congress, Sept. 2023, Bussan, Korea.
- [3] The self-installing package can be free downloaded at <https://temdm.com/msa/>. Its application is discussed in the blog at <https://temdm.com/news>.