Exploring materials with higher acuity electron backscatter diffraction– a combined approach using new machine learning algorithms and direct detectors in the scanning electron microscope

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Electron backscatter diffraction (EBSD) is a now-common technique employed within the scanning electron microscope to capture wide-angle diffraction patterns. These patterns originate from the scattering and diffraction of the scanned electron beam and the crystal lattice. This means that each pattern contains significant information regarding the structure and chemistry of the crystal. In an EBSD experiment, many patterns are captured together and analysed to create rich microstructural maps. The majority of existing approaches for EBSD detection and analysis use serial capturing of the diffraction patterns using an inefficient scintillator-lens-CCD/CMOS detector, and typically each pattern is analysed independently to create insight.

First, we will introduce the benefits of using a direct electron detector based upon a Timepix 3 sensor [1] (similar to prior work of [2]) and how we can compare these with dynamical simulations, generated with Bruker DynamicS. This reveals that the direct electron detector results in diffraction patterns with a higher optical quality, which indicates that more subtle features can be observed.

Next, we will introduce how we can use machine learning techniques to obtain new insight into the structure of materials. This includes two approaches: (1) classification of phases based upon convolutional neural networks [1]; (2) clustering of similar patterns, using non-negative matrix factorisation (NMF), principal component analysis (PCA) and use of an autoencoder [3]. The improved quality of the second approach enables us to analyse the diffraction patterns 'on the sphere' and to resolve the difference between γ and γ' with 'spherical-angular dark field imaging', from integrated band profiles of specific lattice planes [2].

[1] A.F. Foden, A. Previero, and T.B. Britton *Advances in electron backscatter diffraction* https://arxiv.org/abs/1908.04860

[2] S. Vespucci, A. Winkelmann, G. Naresh-Kumar, K. P. Mingard, D. Maneuski, P. R. Edwards, A. P. Day, V. O'Shea, and C. Trager-Cowan *Digital direct electron imaging of energy-filtered electron backscatter diffraction patterns* Phys. Rev. B (2015)

[3] T.P. McAuliffe, D. Dye, and T.B. Britton *Spherical-angular dark field imaging and sensitive microstructural phase clustering with unsupervised machine learning* https://arxiv.org/abs/2005.10581