ADVANCING PATTERN ANALYSIS

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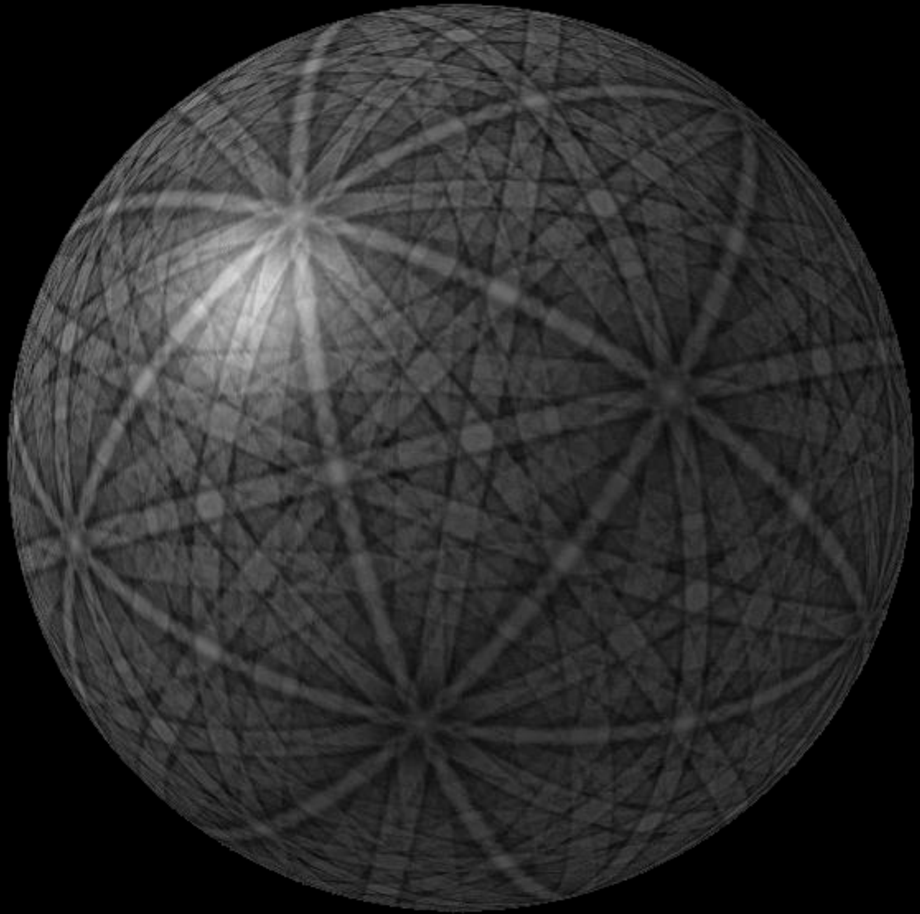


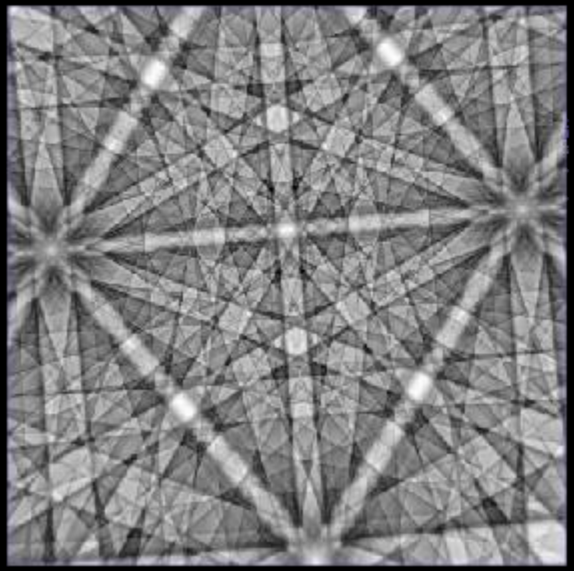
@bmatb

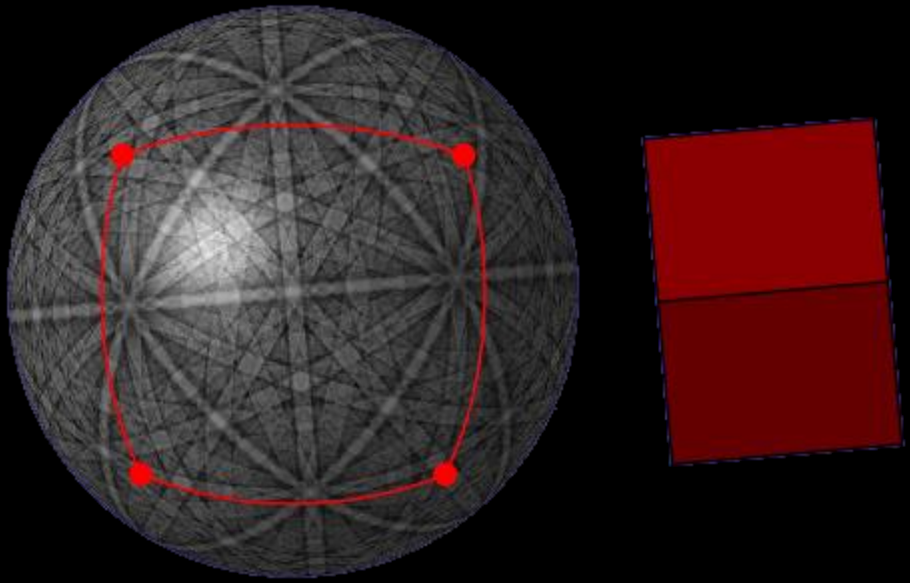
MOTIVATION

- Conventional EBSD is inviable for characterisation
  - Fast
  - Information rich
  - ‘Robust’

- Dynamical EBSD pattern simulation now available

- Can we improve existing approaches?

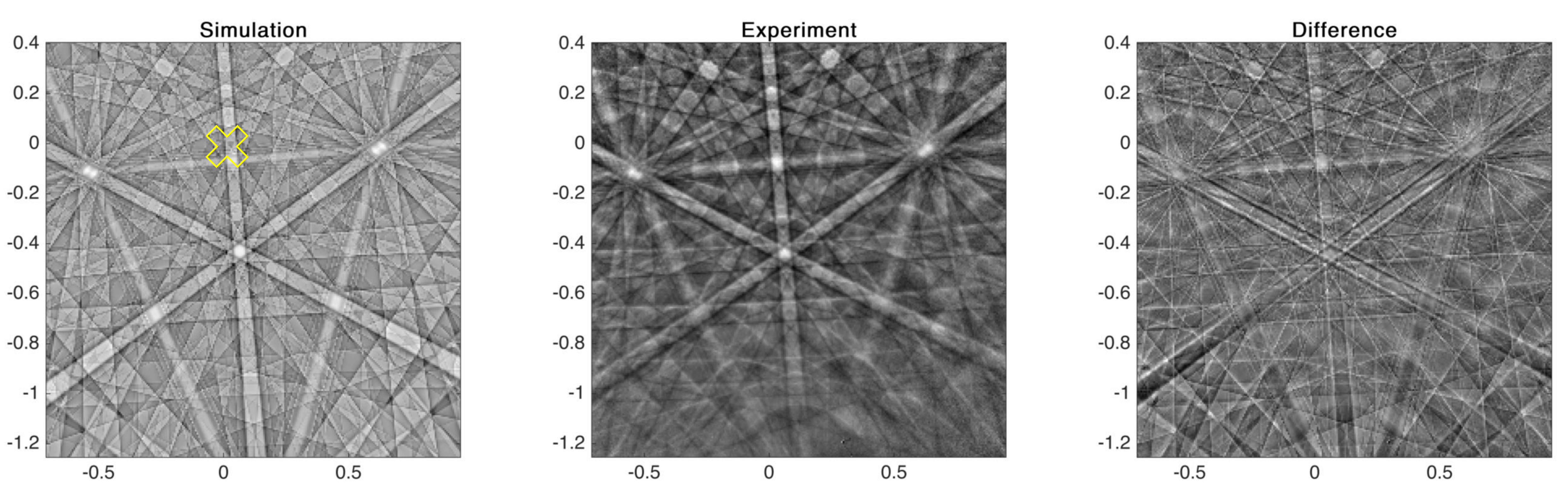




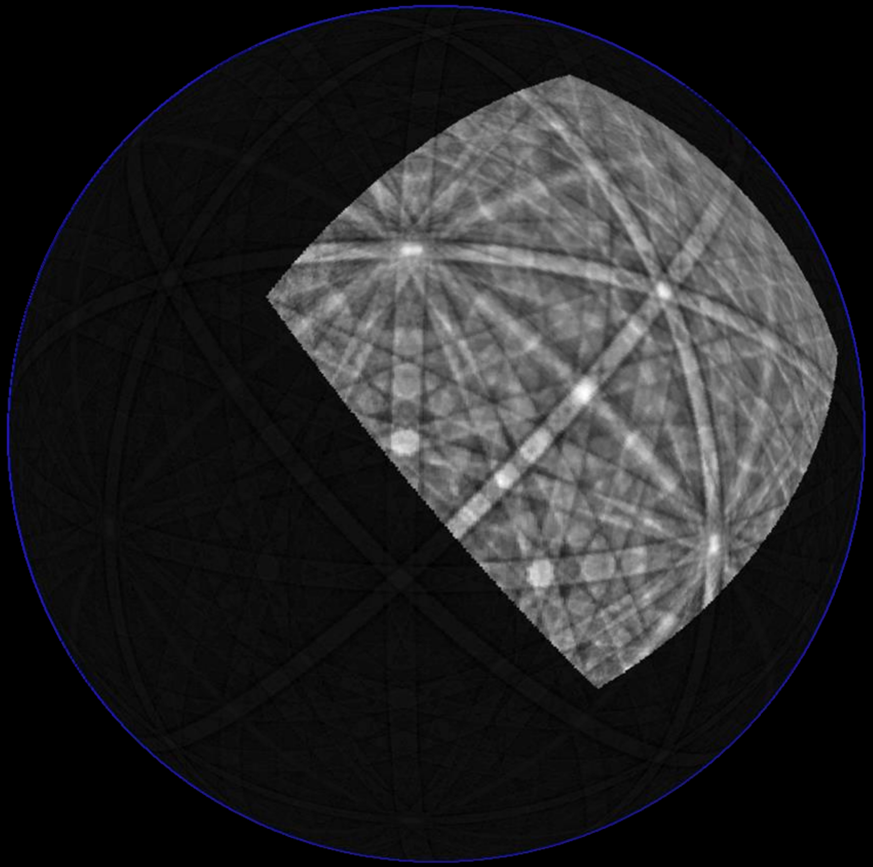
For a more broad introduction to EBSD, see - https://www.youtube.com/playlist?list=PLo_ZiAxtCLkqaujdC4pnAF7_rmQ0bPiqT

DIRECT ELECTRON DETECTION (DED)

Simulation from (reprojected) from Bruker Dynamics



‘NEW’ APPROACHES

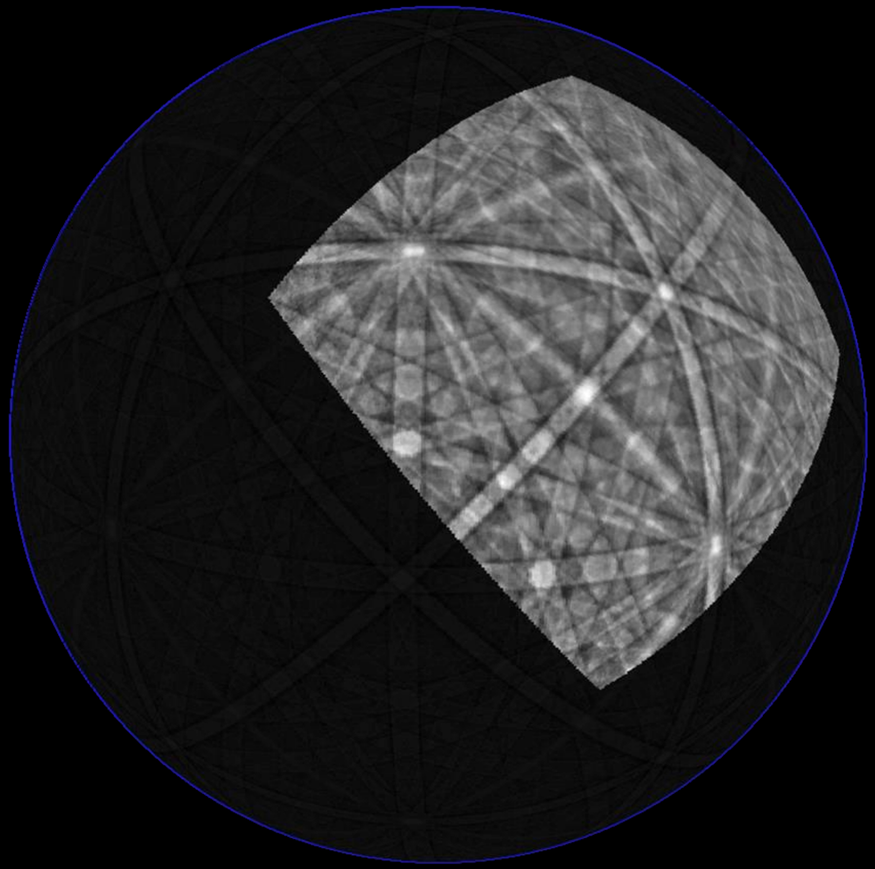


Apply 24 symmetries

Single pattern on sphere

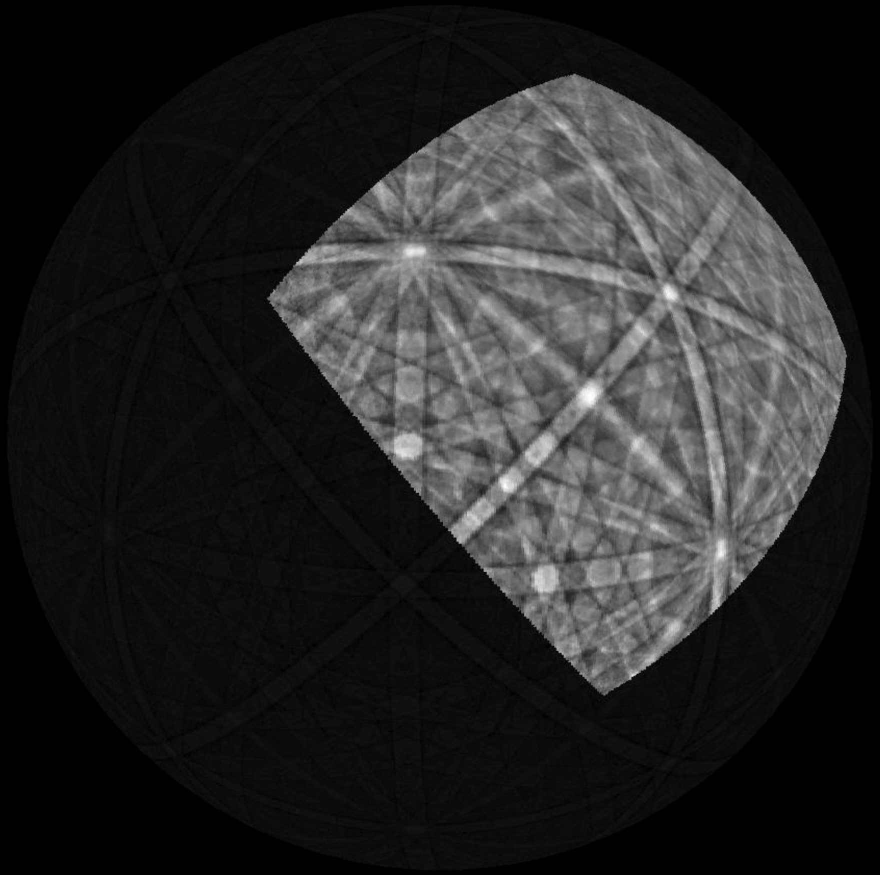
Britton et al. (2019) https://arxiv.org/abs/1908.04860

'NEW' APPROACHES



Single pattern on sphere

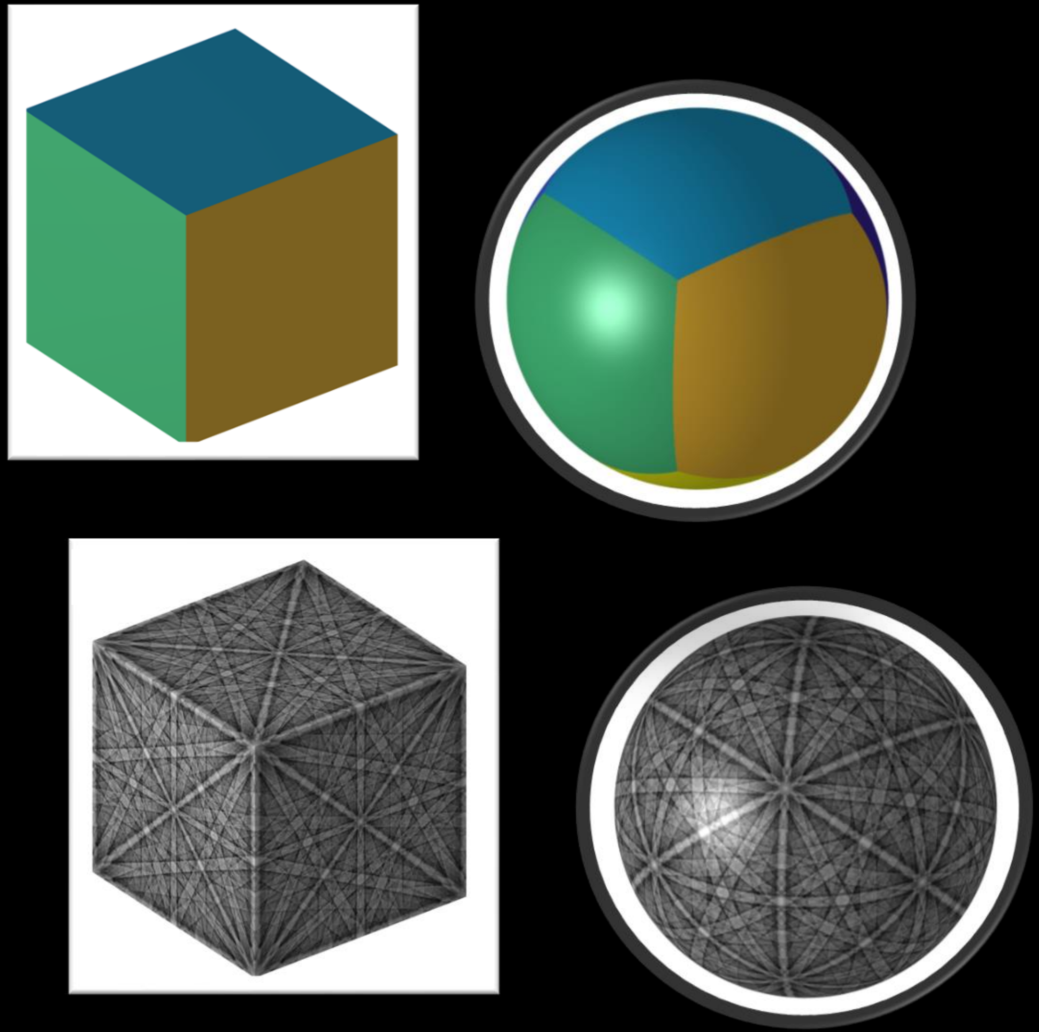
Apply 24 symmetries



Application of symmetry and coverage of sphere

CHALLENGE

- Can we utilise spherical projections [1] to understand Kikuchi patterns?
- Use dynamical patterns [2] to develop routines & apply to experiments
- Use the spherical harmonic functions in MTEX

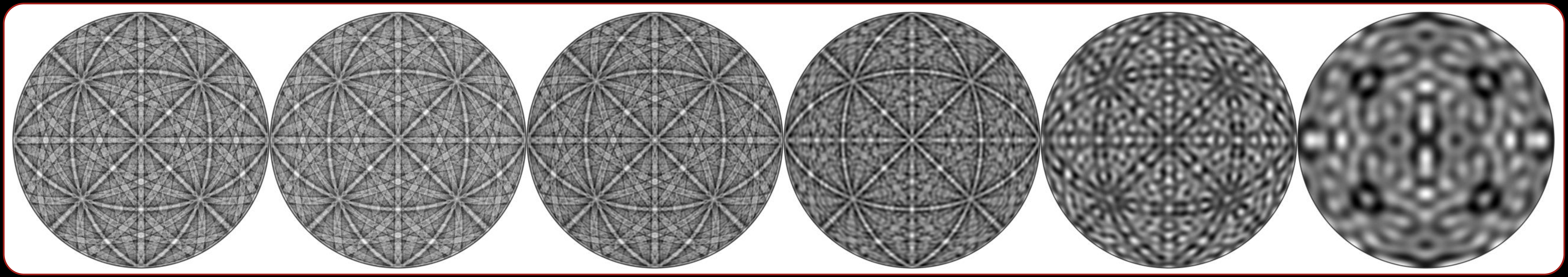


[1] A. Day J. of Microscopy (2008)
[2] A. Winkelmann et al. Ultramicroscopy (2007)

FFT APPROXIMATION

- Approximate the EBSD pattern on the surface of the sphere
- Use non equispaced fast Fourier transform (available in MTEX)

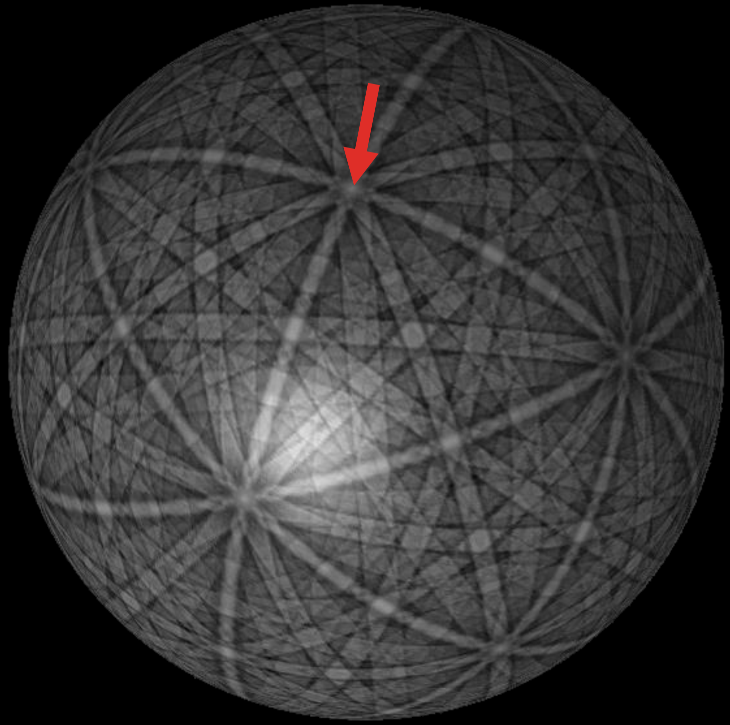
Increased approximation →

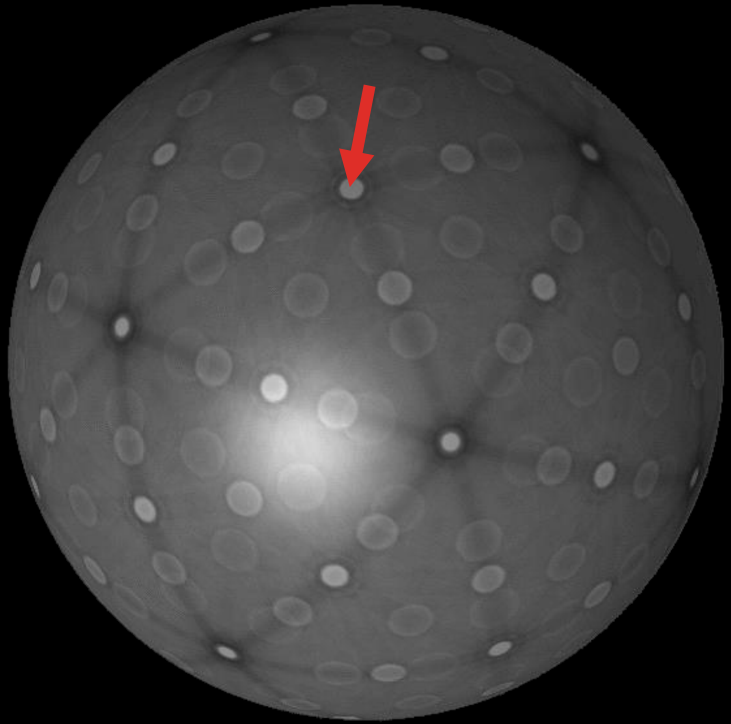


Original | N = 512 | 256 | 128 | 64 | 32

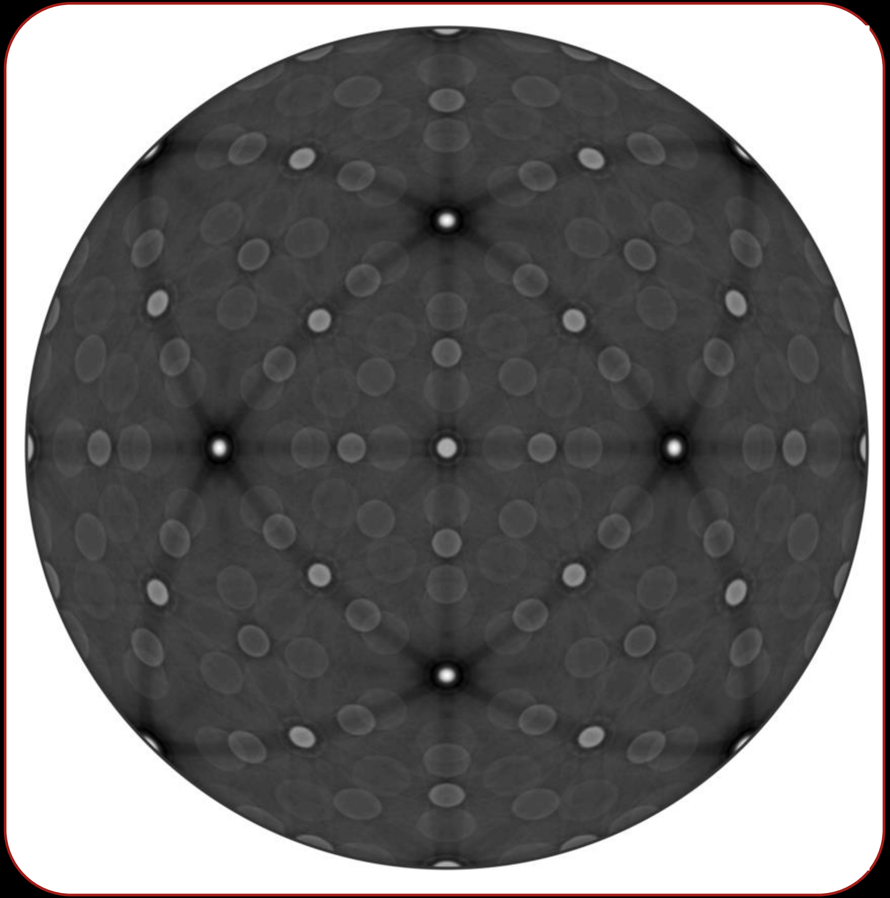
RADON TRANSFORMS

- The Radon transform is related to the Fourier transform
- Transform the sFFT to the sRadon
    - Planes become spots
    - Structure of the spots = characteristic of each band

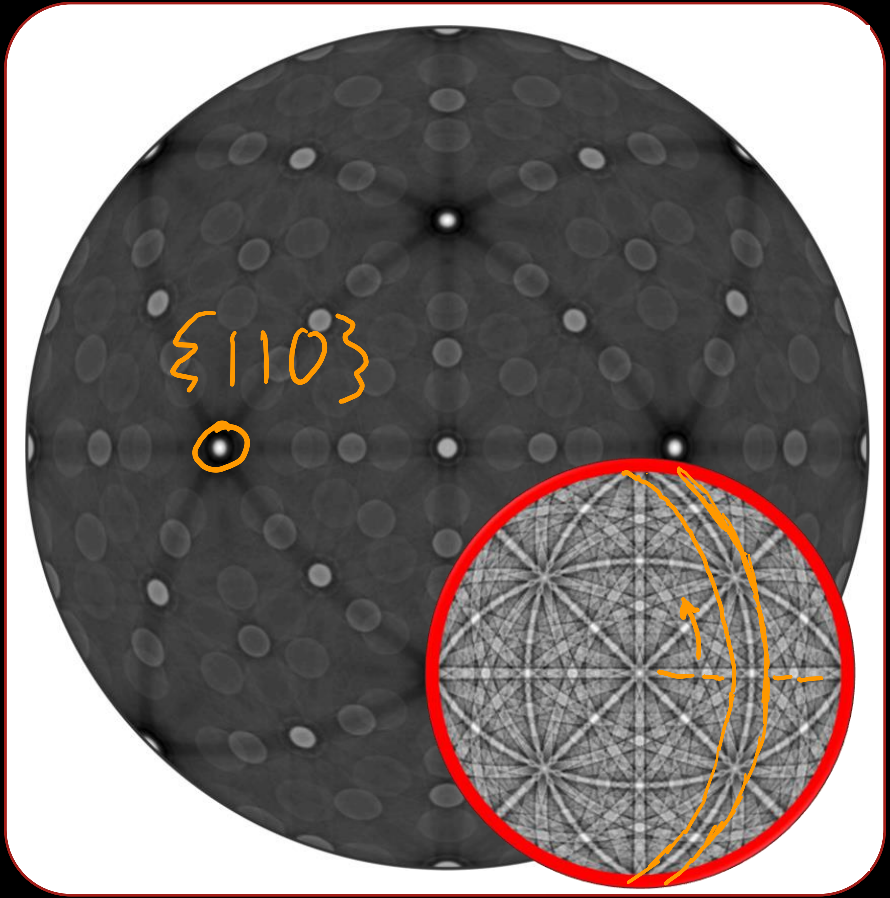




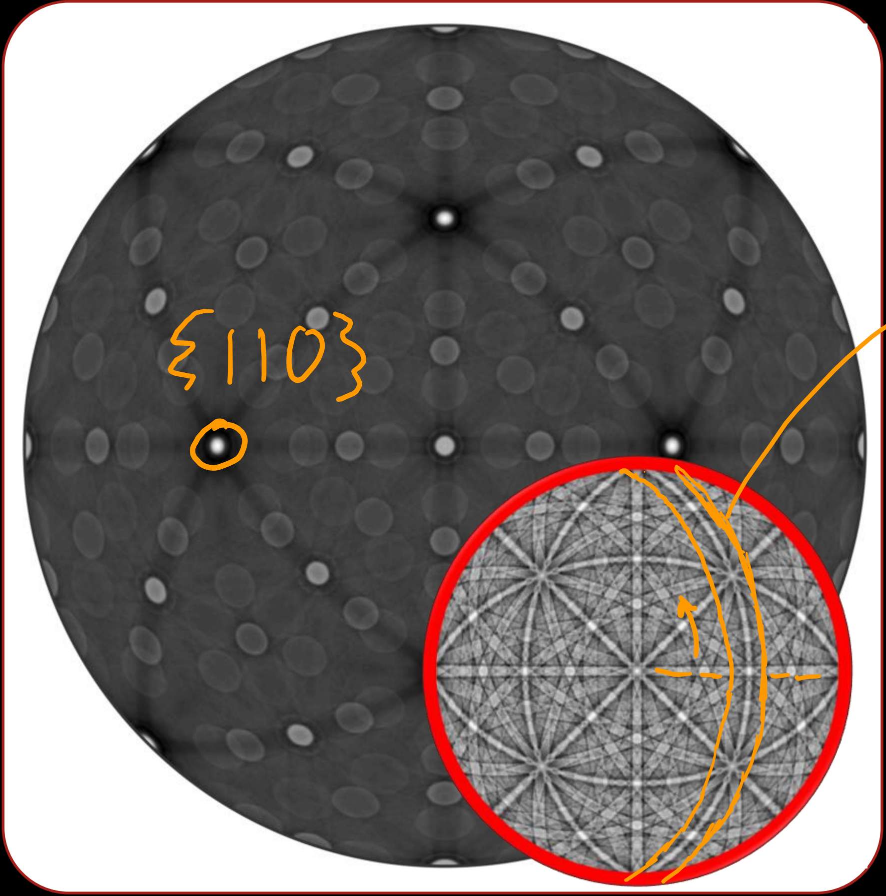
BAND PROFILE EXTRACTION

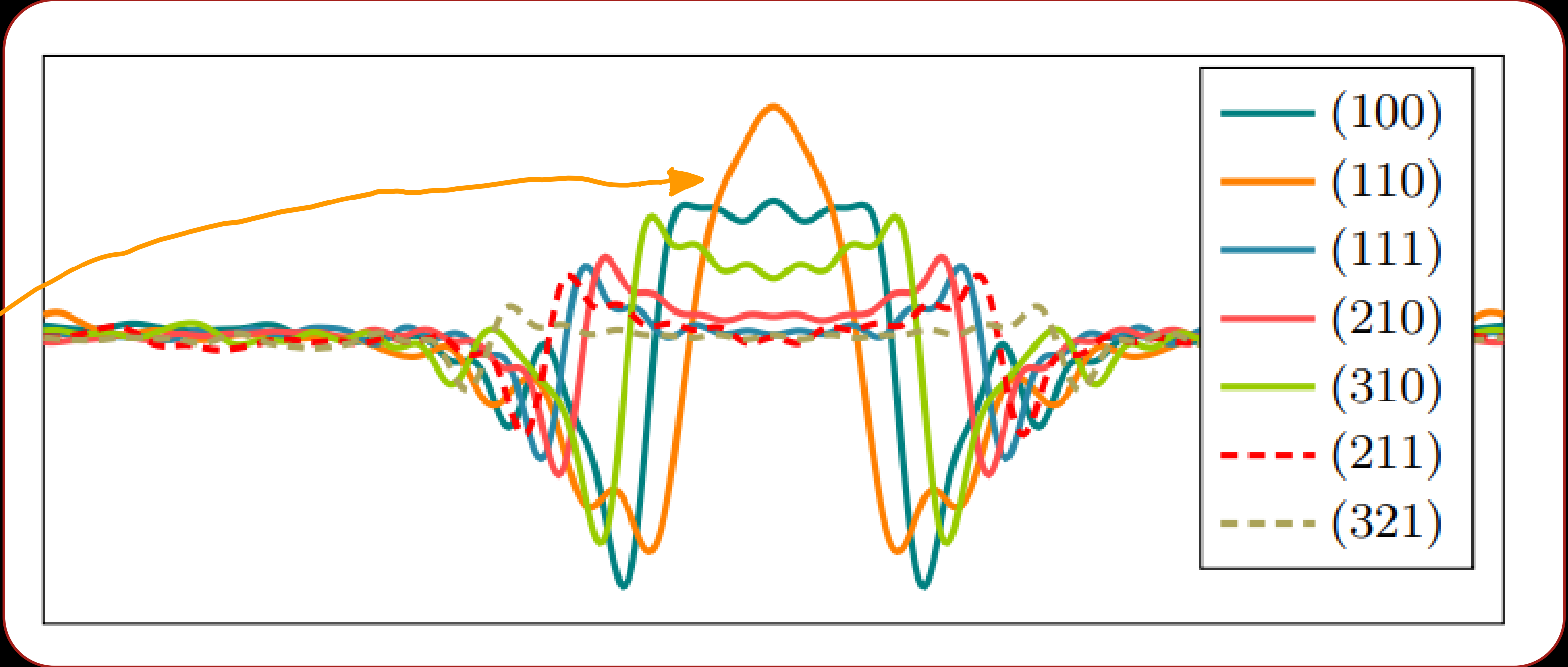


BAND PROFILE EXTRACTION



BAND PROFILE EXTRACTION

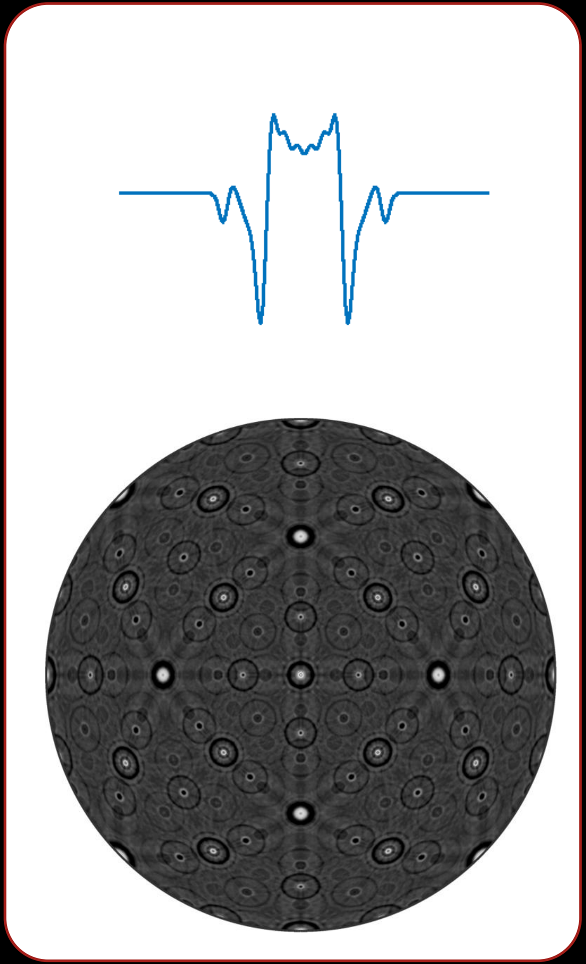


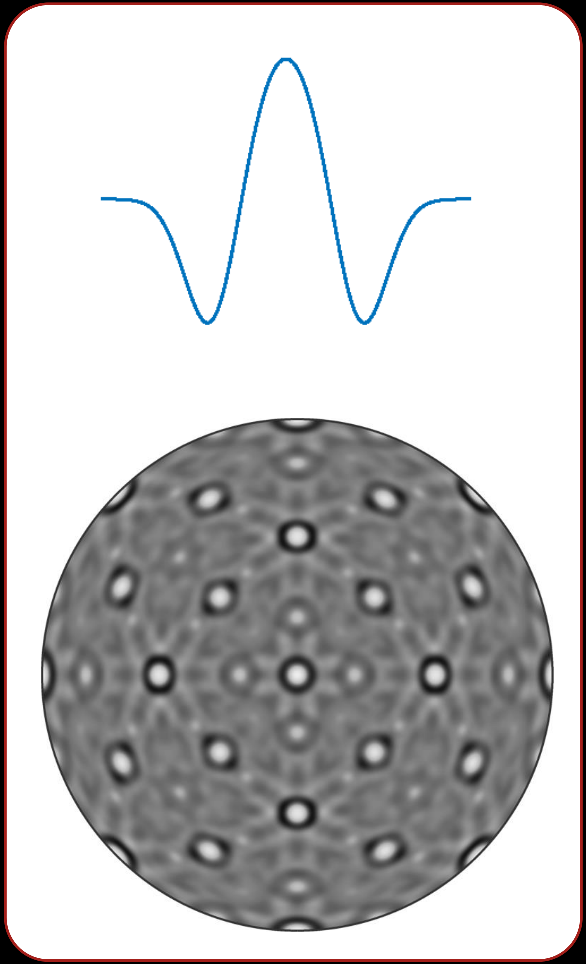


Small circle integrals from the original pattern,
i.e. above and below the great circles,
but performed in the Radon transform

ORIENTATION DETERMINATION

- Spherical Radon → find peaks for each band
- Convolve 'average' profile
  - Structured peak detects structured bands
- Once the peaks are found we can index with AstroEBSD [3]

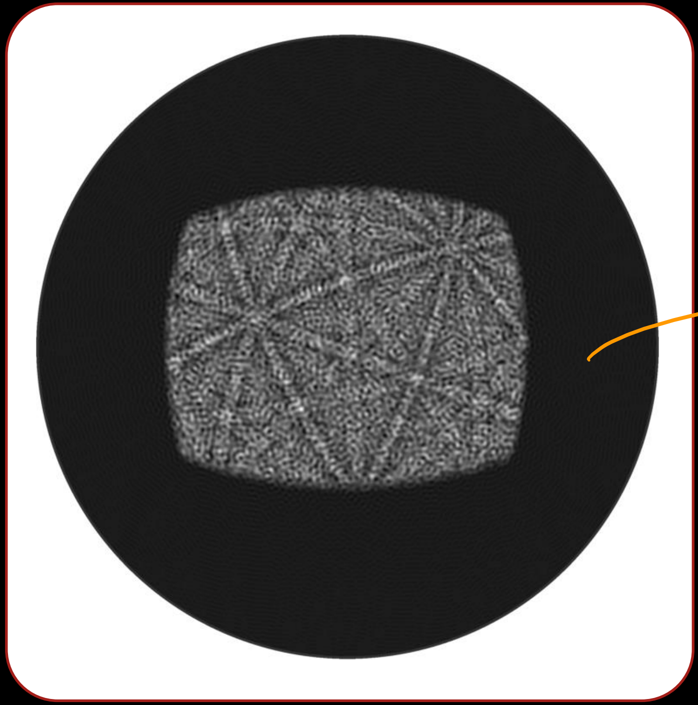




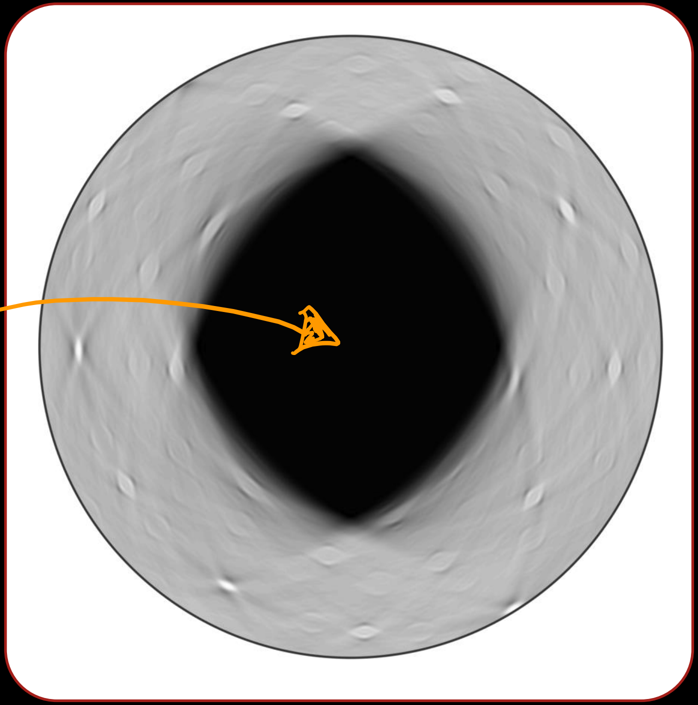
[3] www.github.com/BenjaminBritton/AstroEBSD & Britton et al. IUCR (2018)

PATTERN INCOMPLETENESS

- Real patterns do not subtend the entire sphere
- Window and sFFT approximate
- Radon transform
- Normalise intensities in the Radon transform

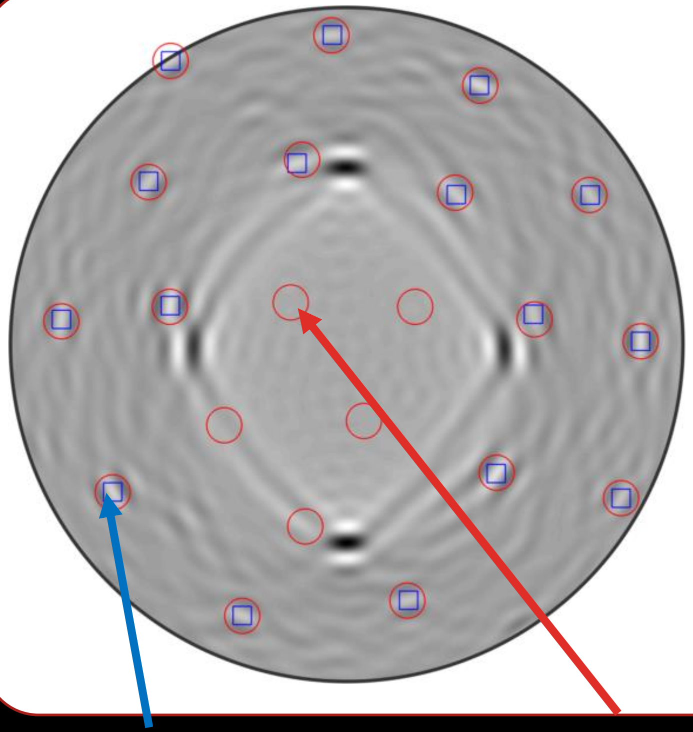


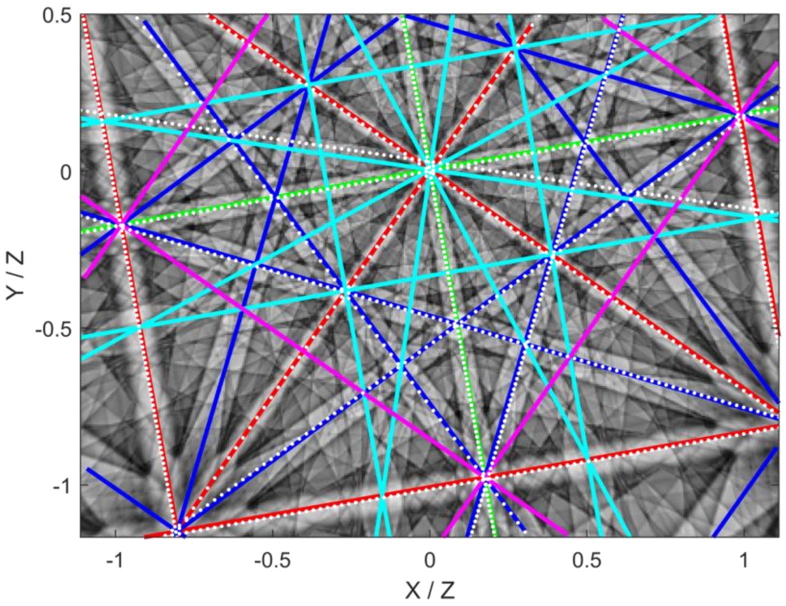
Experimental pattern on sphere, with reduced angle subtended

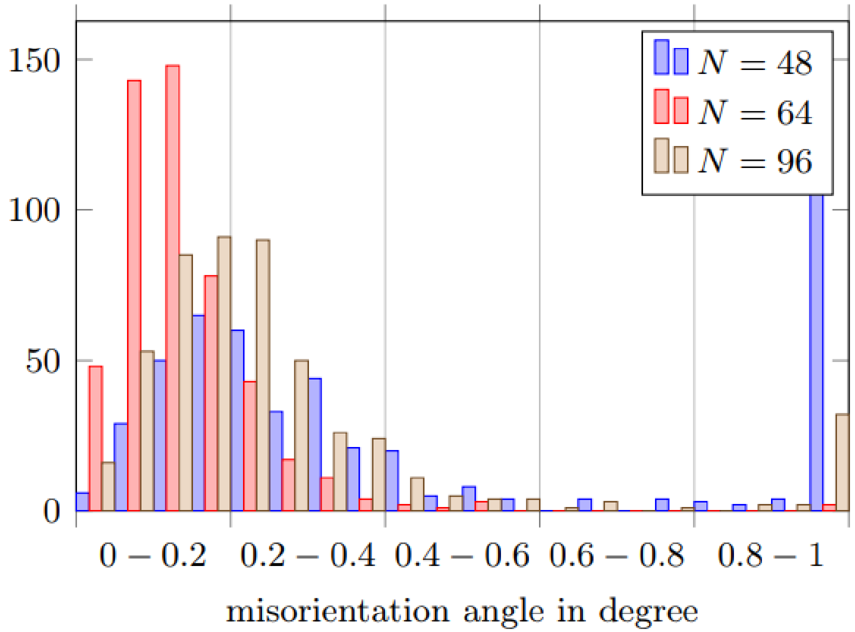


Experimental pattern, on Radon sphere

SPHERICAL RADON - INDEXED PATTERN



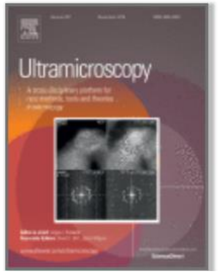




Detected Peaks   Expected Peaks   Measuring true orientations

For orientation conventions, see: Britton et al. (2016) Materials Characterisation
For AstroEBSD: see https://github.com/benjaminbritton/astroebsd & Britton et al (2018) Journal of Applied Crystallography

PATTERN MATCHING

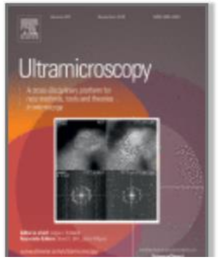


Ultramicroscopy

Volume 207, December 2019, 112836

Gazing at crystal balls: Electron backscatter diffraction pattern analysis and cross correlation on the sphere

Ralf Hielscher [a], Felix Bartel [a], Thomas Benjamin Britton [b]



Ultramicroscopy

Volume 207, December 2019, 112845

Indexing electron backscatter diffraction patterns with a refined template matching approach

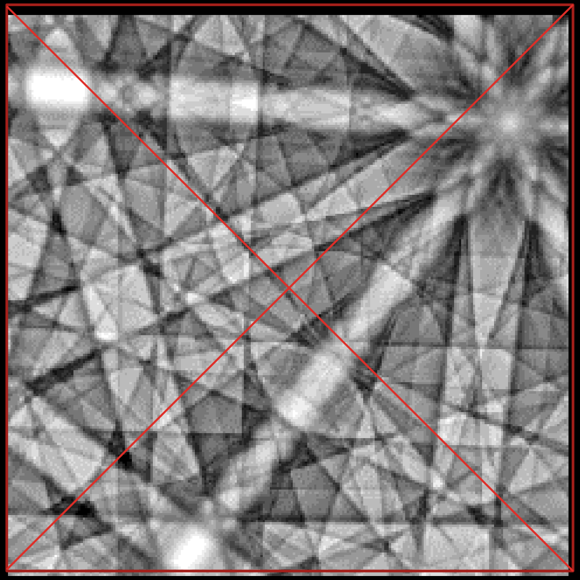
A. Foden [a], D.M. Collins [b, c], A.J. Wilkinson [b], T.B. Britton [a]

Other variants are available (e.g. dictionary indexing)

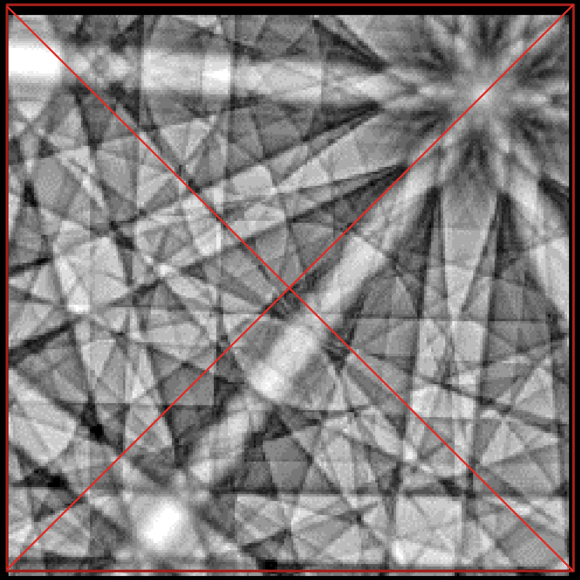
2D CROSS CORRELATIONAL

$$\chi_d = \frac{\sum_i [(x[i] - \bar{x}) \cdot (y[i-d] - \bar{y})]}{\sqrt{\sum_i (x[i] - \bar{x})^2} \sqrt{\sum_i (y[i-d] - \bar{y})^2}}$$

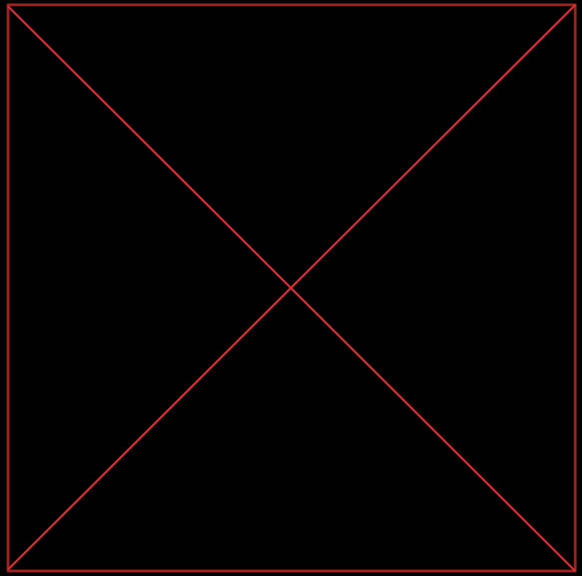
[X = 1 , Y= 1]



Reference



Test



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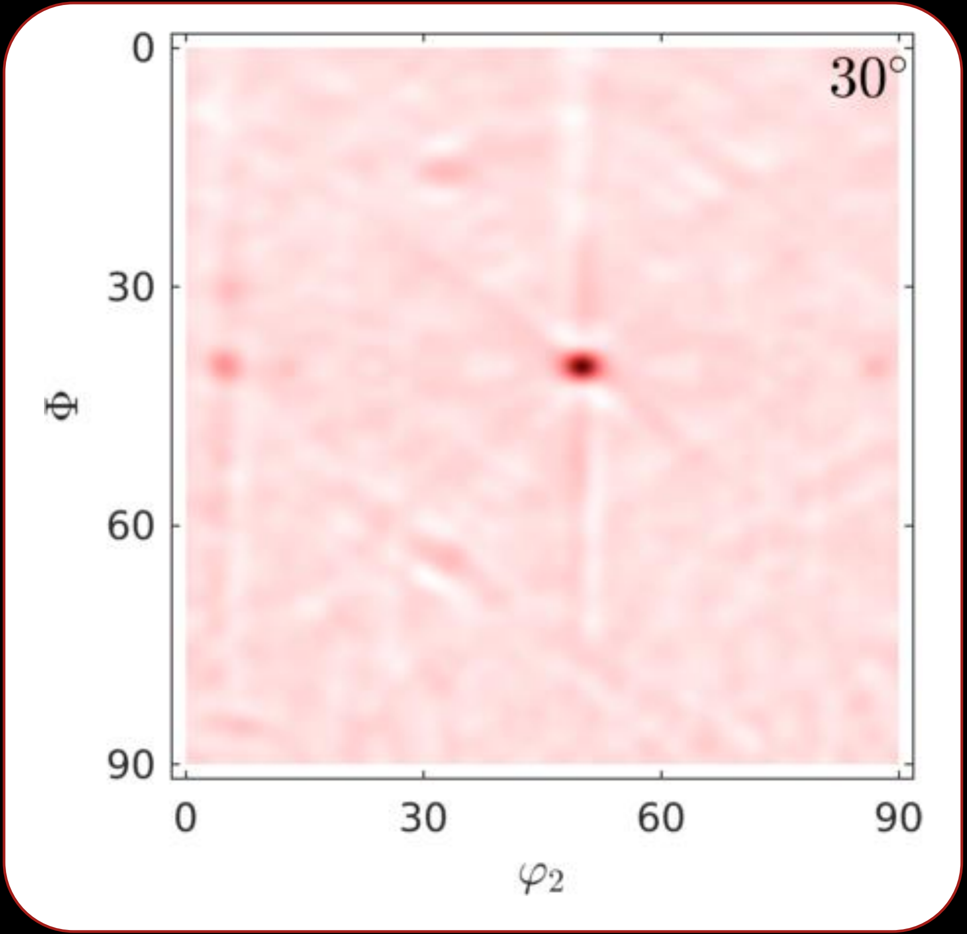
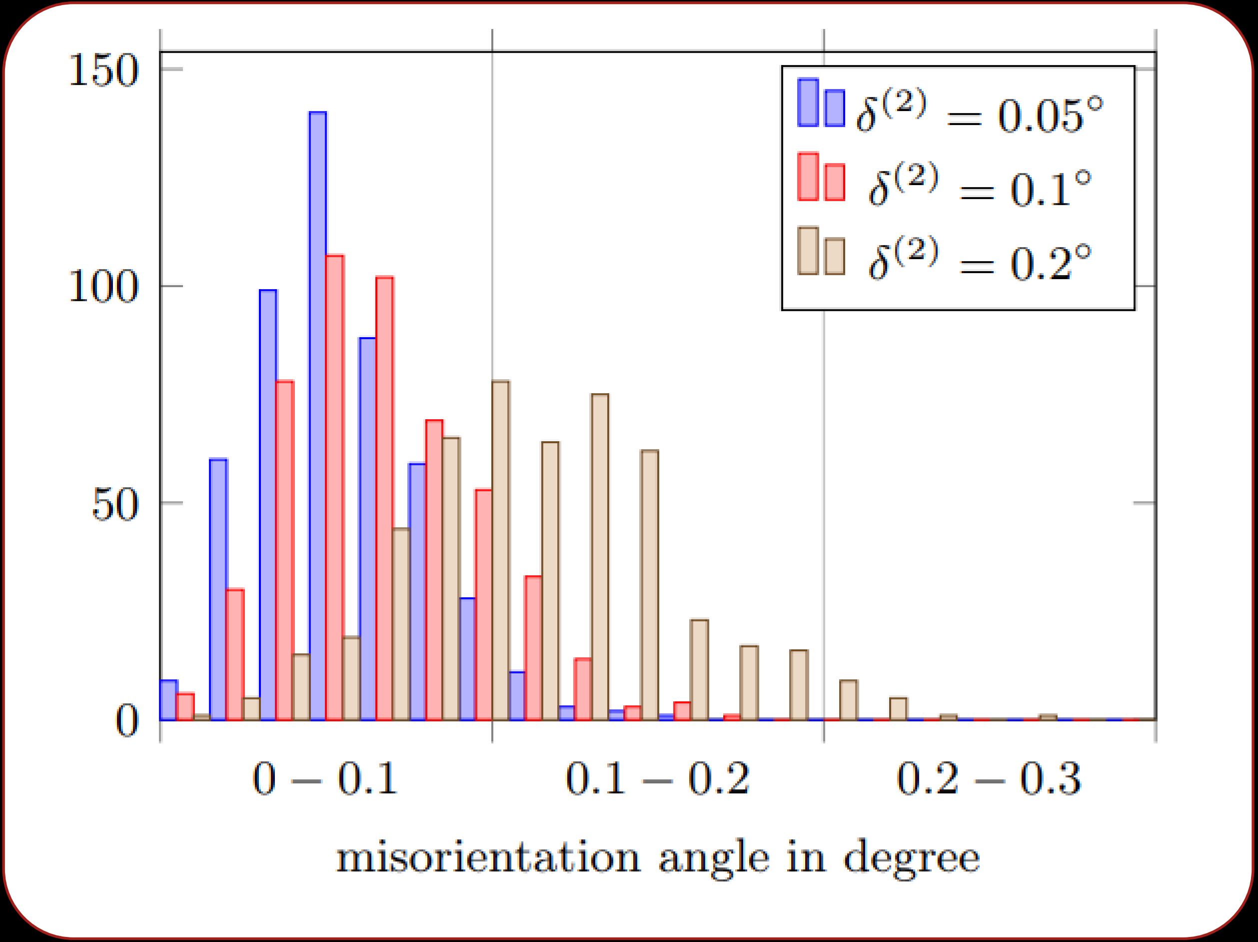
3D SPHERICAL CROSS CORRELATION

- Experimental and simulated pattern are both in Fourier space
- Parameterise the sFFT for correlation peak correlated to components of the misorientation [i.e. SO(3)]
- Correlation precision prop. to sFFT bandwidth
    - Use hierarchical grid for final search



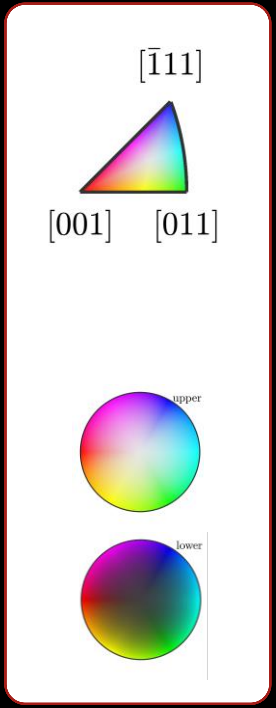
RESOLUTION AND TIME



- Cut off N = 64
- Points on M1 for 1.5° = 180,000
- Radius of upsample = 1.5°
- Points on M2 for 0.05° = 110,000
- Speed = 1/second (multicore)

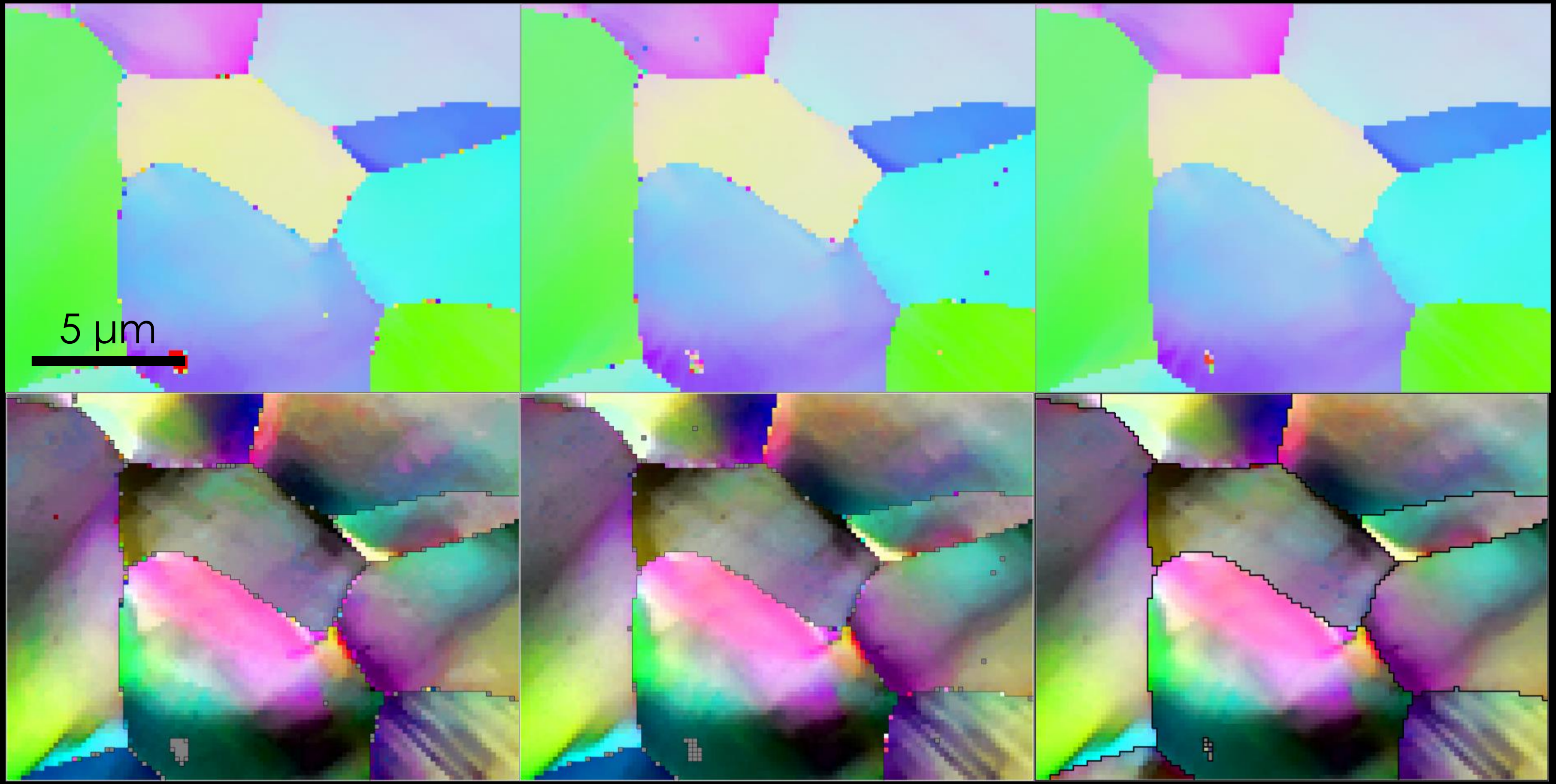
MAP COMPARISON

w.r.t. IPF-horizontal colourmap



Axis w.r.t. mean per grain 5° radius

2D + Astro | Sphere + Astro | Sphere + XCF

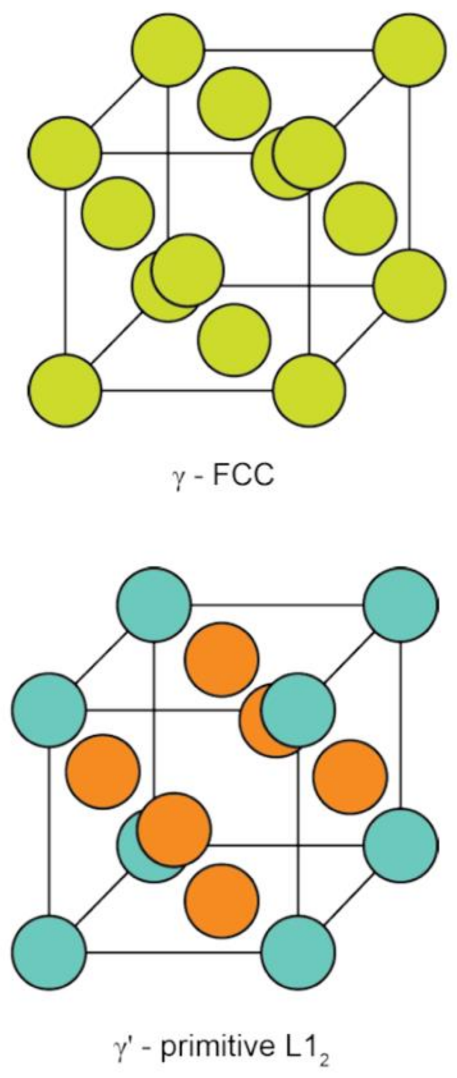


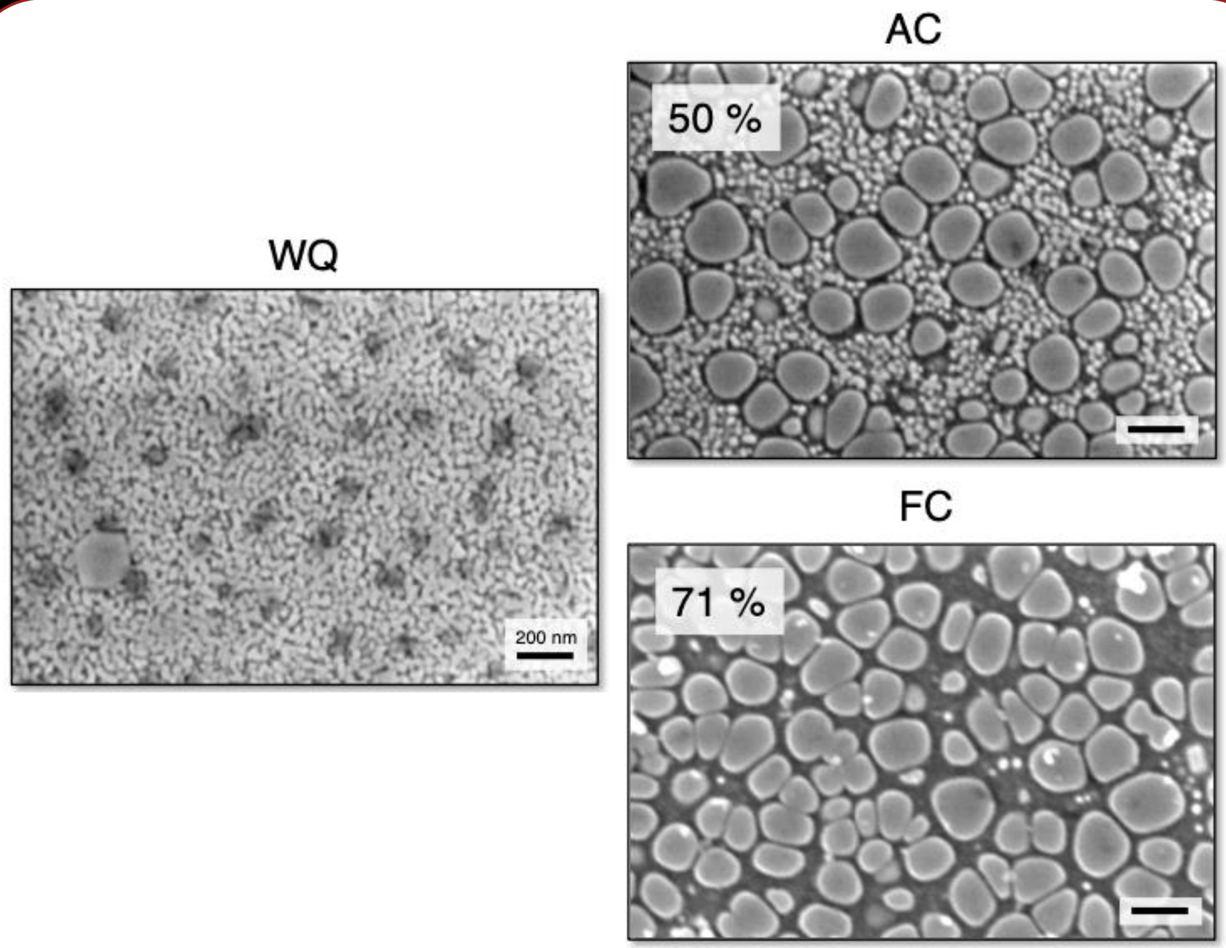
McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132

SPHERICAL-ANGULAR DARK FIELD IMAGING & PHASE CLUSTERING WITH MACHINE LEARNING

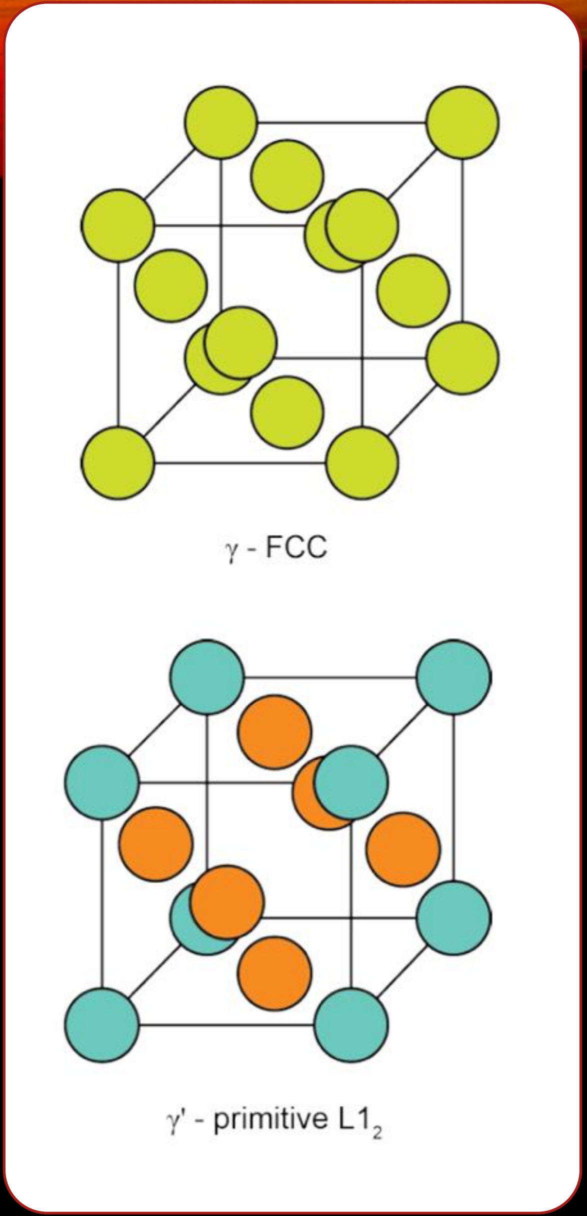
Thomas P McAuliffe, David Dye, T Ben Britton

ANALYSIS OF GAMMA/GAMMA'



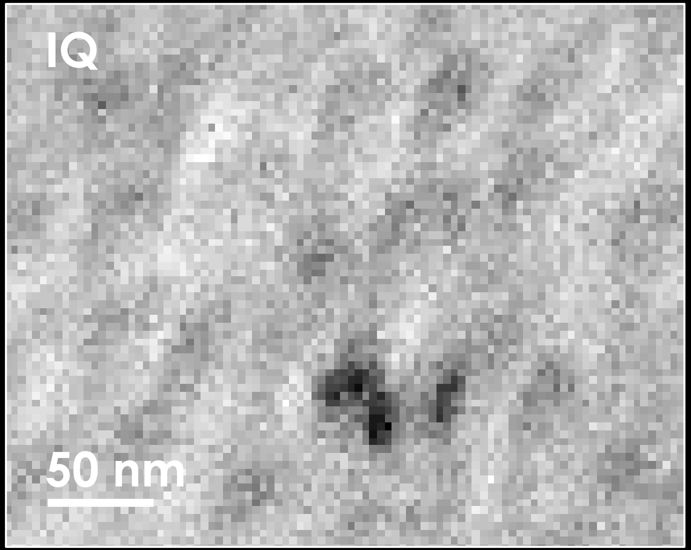


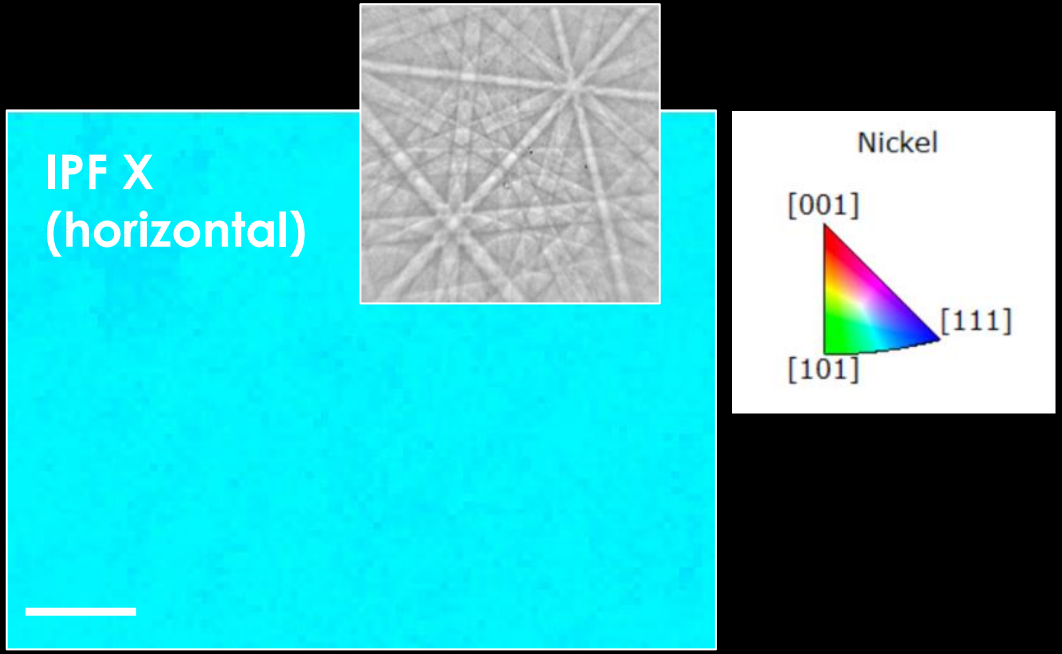
Tom P. McAuliffe, unpublished data



- Not much information in Band location information (IQ from Hough transform).

- Cluster the patterns into self-similar categories using EBSPs.





McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132

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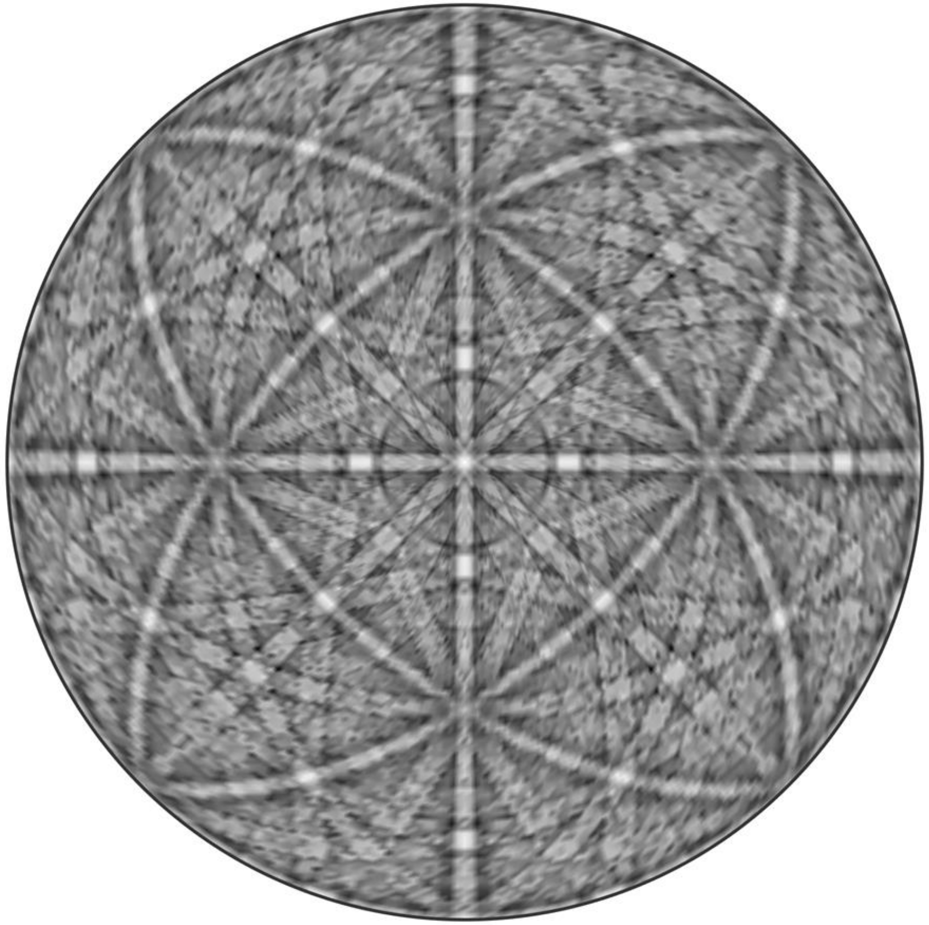
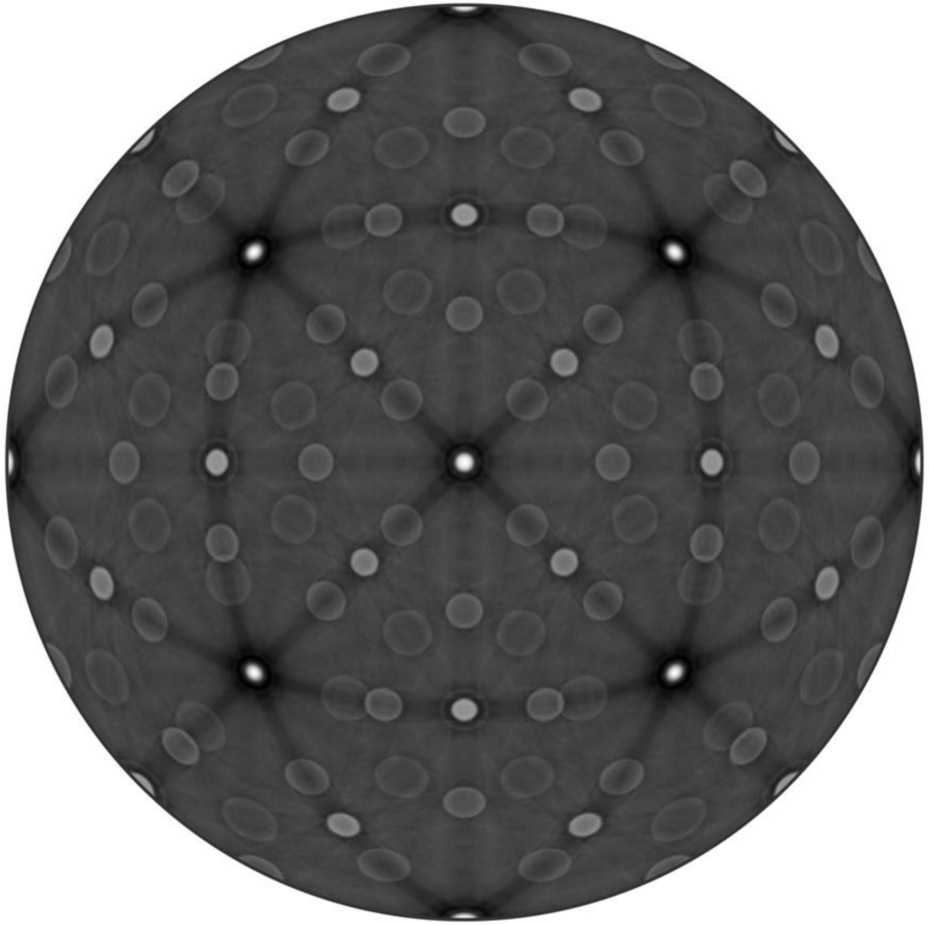
For dynamical EBSD patterns we observe **some structural differences** but no systematic band absences...

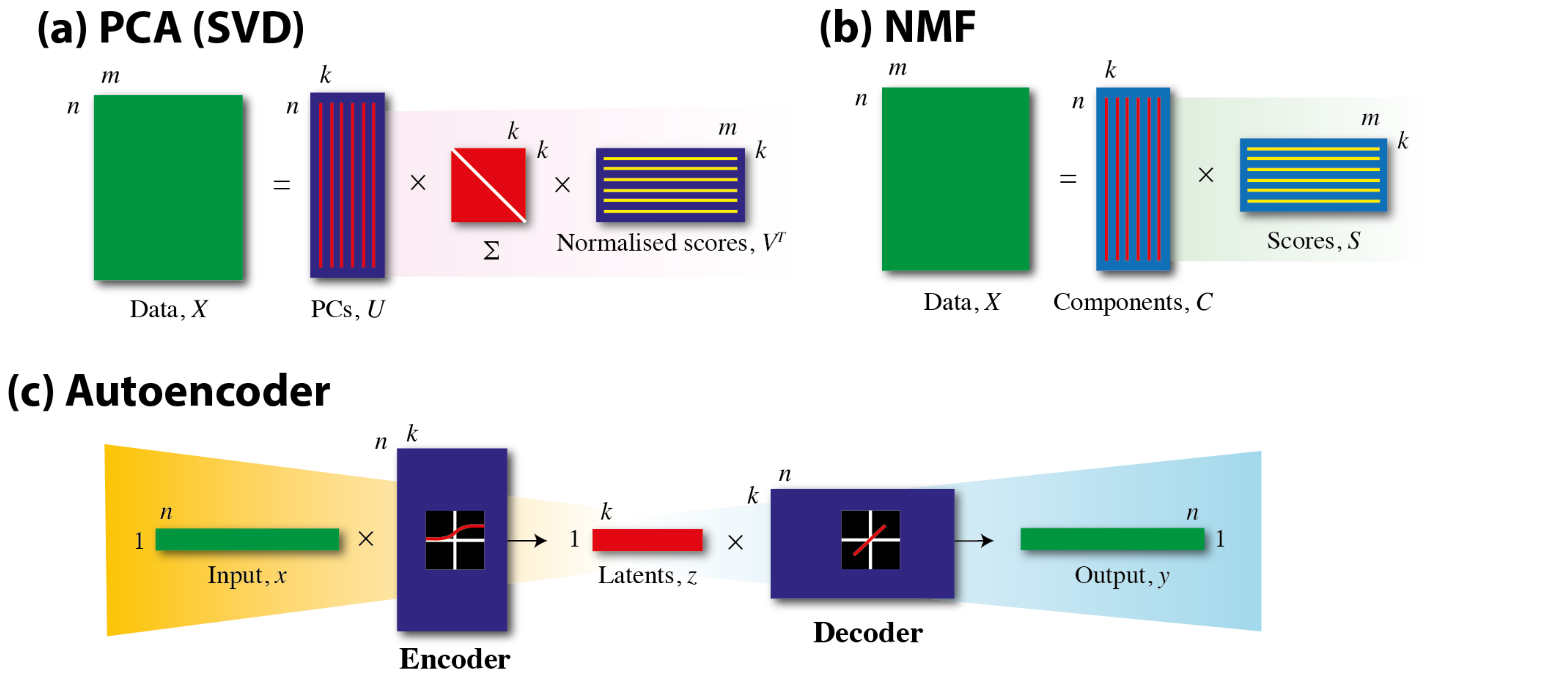


Dynamically simulated EBSP



Spherical radon transform

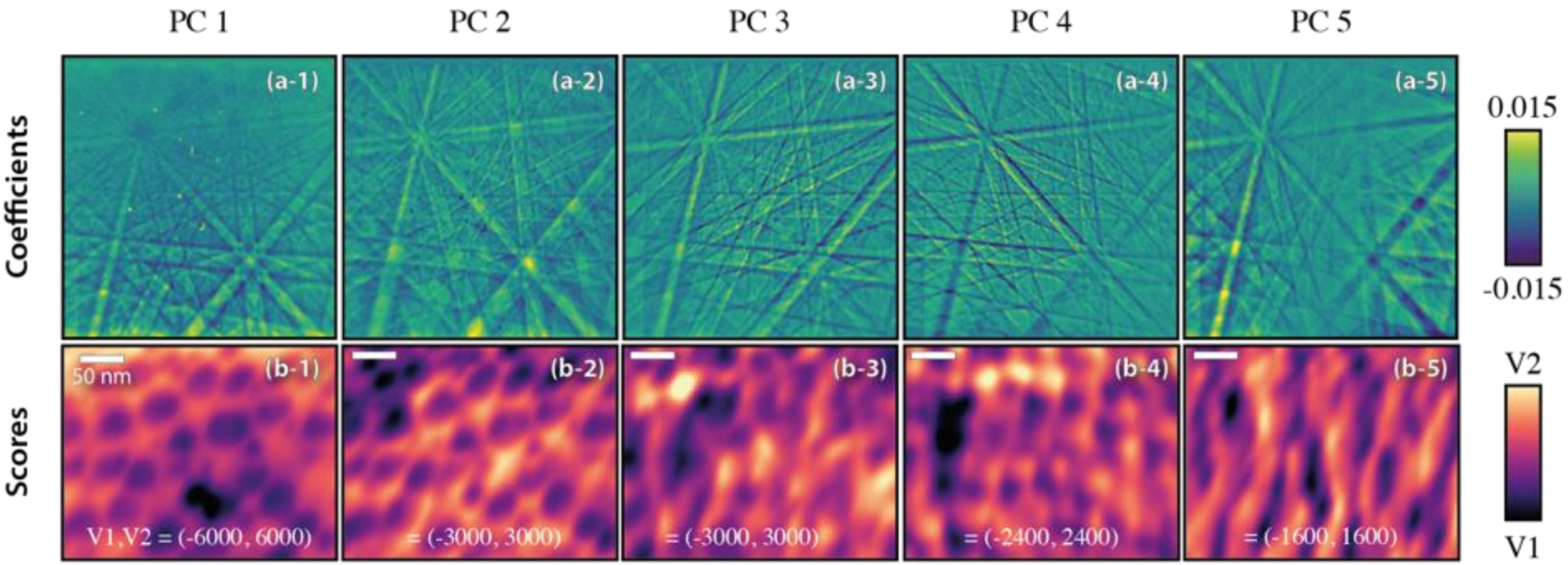
McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132

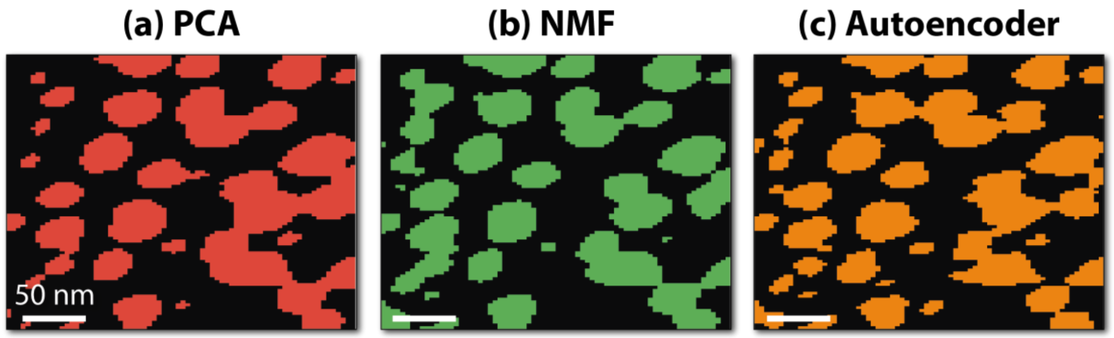


- Use three approaches for looking at latent features of a dataset.
- All give '**factors**': the underlying base signals in the dataset - form a basis for approximating data.
- All give '**scores**': how well a latent factor represents a data point.

McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132

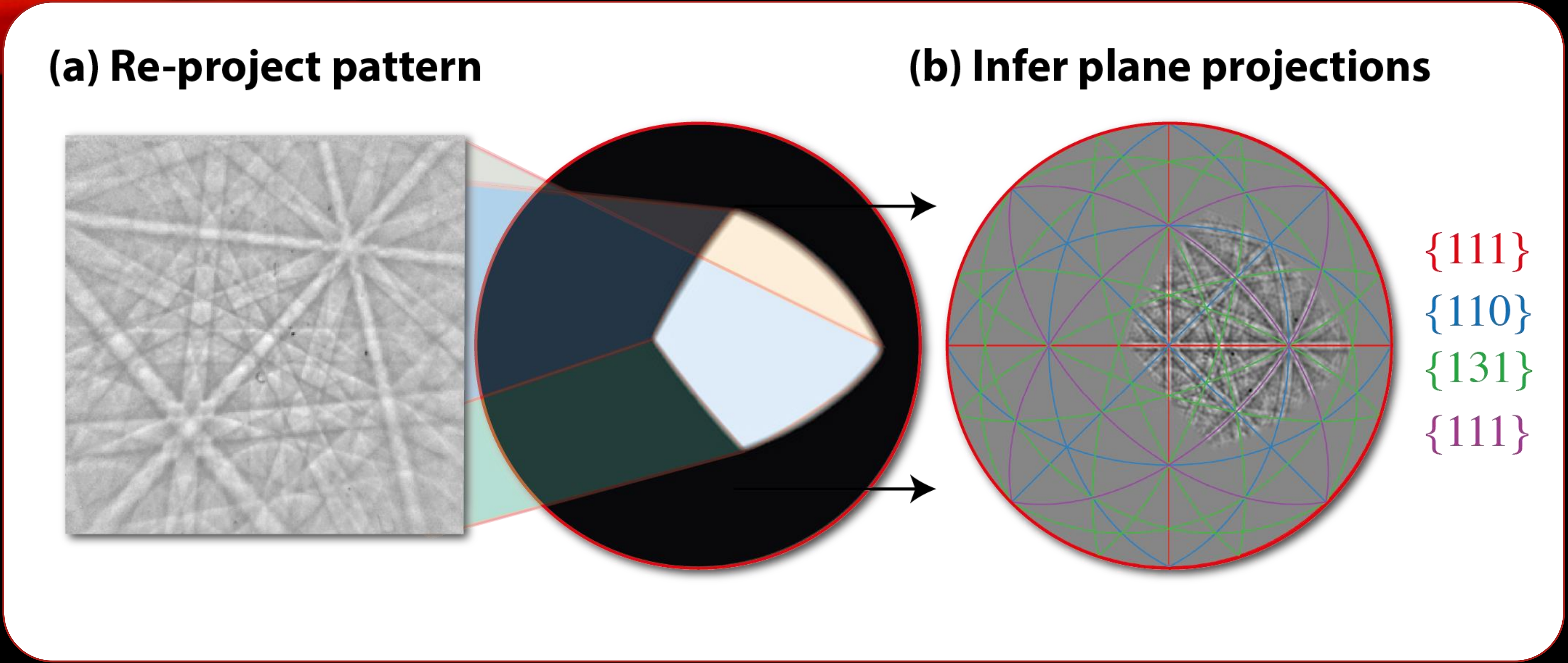
Principal Component Analysis





- Segmenting on these scores gives good phase discrimination

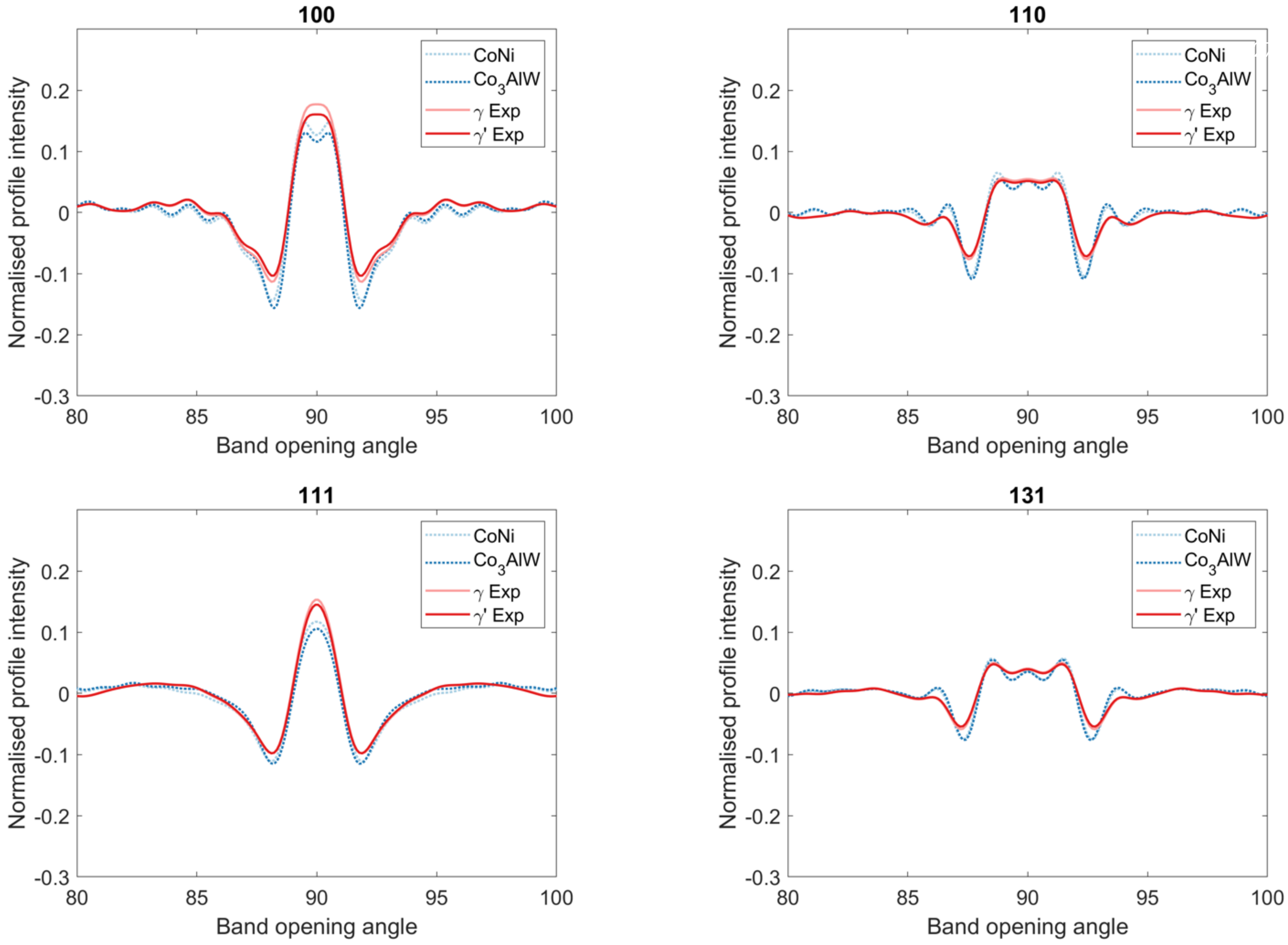
McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132



- Use spherical harmonics to project an EBSP back onto the diffraction sphere
- Then quantitatively compare experimental or representative dataset factor patterns with simulations.

McAuliffe et al. https://arxiv.org/abs/2005.10581 & [10.1016/j.ultramic.2020.113132](https://doi.org/10.1016/j.ultramic.2020.113132)

Average patterns from segmented regions



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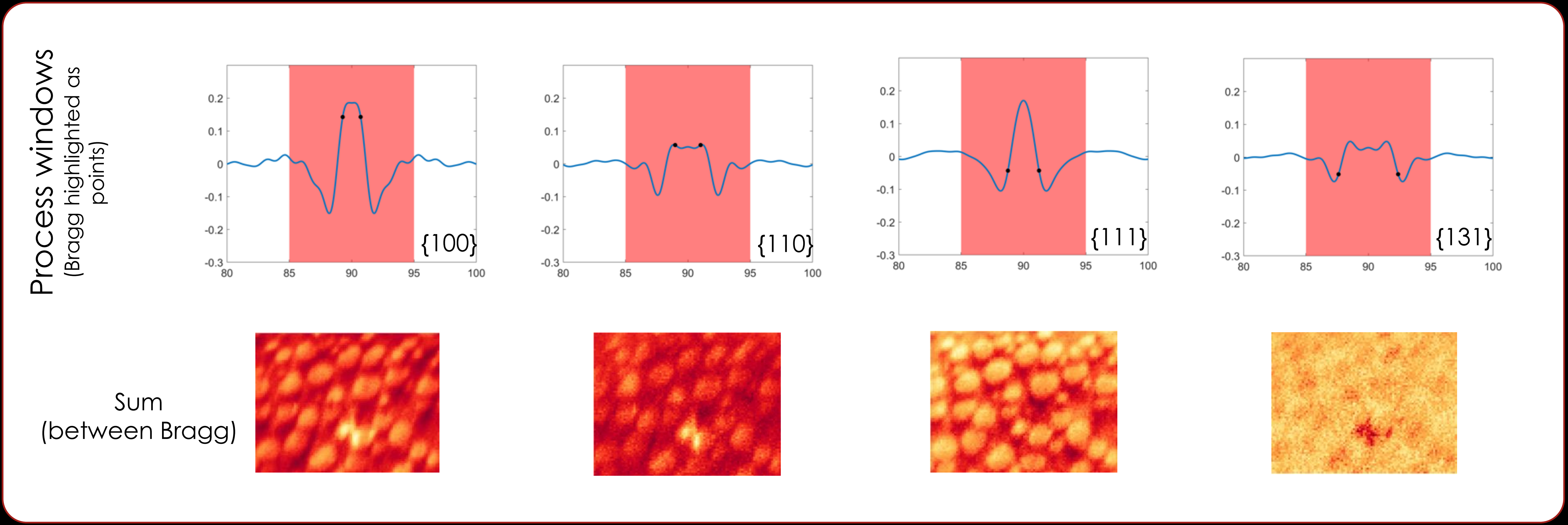
SPHERICAL-ANGULAR DARK FIELD IMAGING



- Use virtual aperture (on each band) to create maps
- *sum* intensity between Bragg points (shown as dots)

McAuliffe et al. https://arxiv.org/abs/2005.10581 & 10.1016/j.ultramic.2020.113132

CODES ALL OPEN SOURCE

- Spherical pattern matching within MTEX
- Spherical radon within MTEX
- (Gnomonic) Pattern processing in AstroEBSD (https://github.com/benjaminbritton/AstroEBSD)
- Statistical clustering in AstroEBSD & python tools (amplify signal to noise)
- See:
  - Hielscher et al. (2019) Ultramicroscopy https://arxiv.org/abs/1810.03211
  - McAuliffe et al. (2020) Ultramicroscopy https://arxiv.org/abs/2005.10581
  - https://tmcauliffe.medium.com/quantitative-microstructural-characterisation-with-astroebsd-2380650c1243


ANY QUESTIONS?
www.expmicromech.com