Three-dimensional Full-field X-ray Orientation Microscopy

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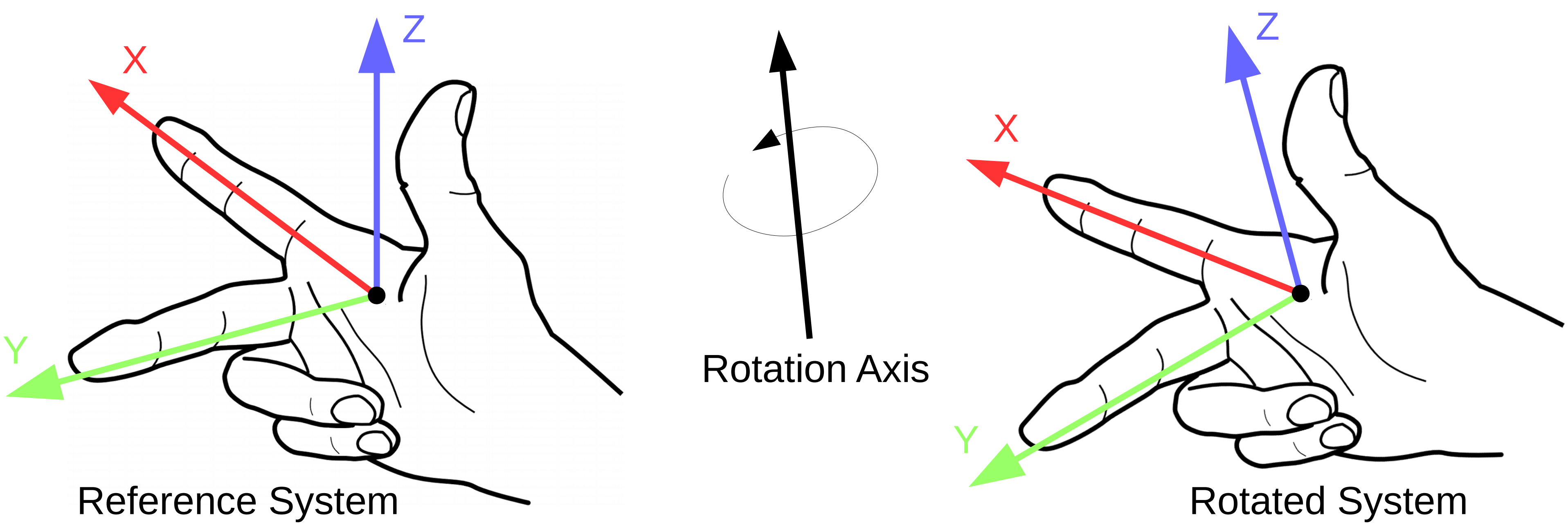
Wait! Local “orientation”, uhm... what?

- Crystallographic Orientation:

  “Relationship between the crystal coordinate system and a reference coordinate system”

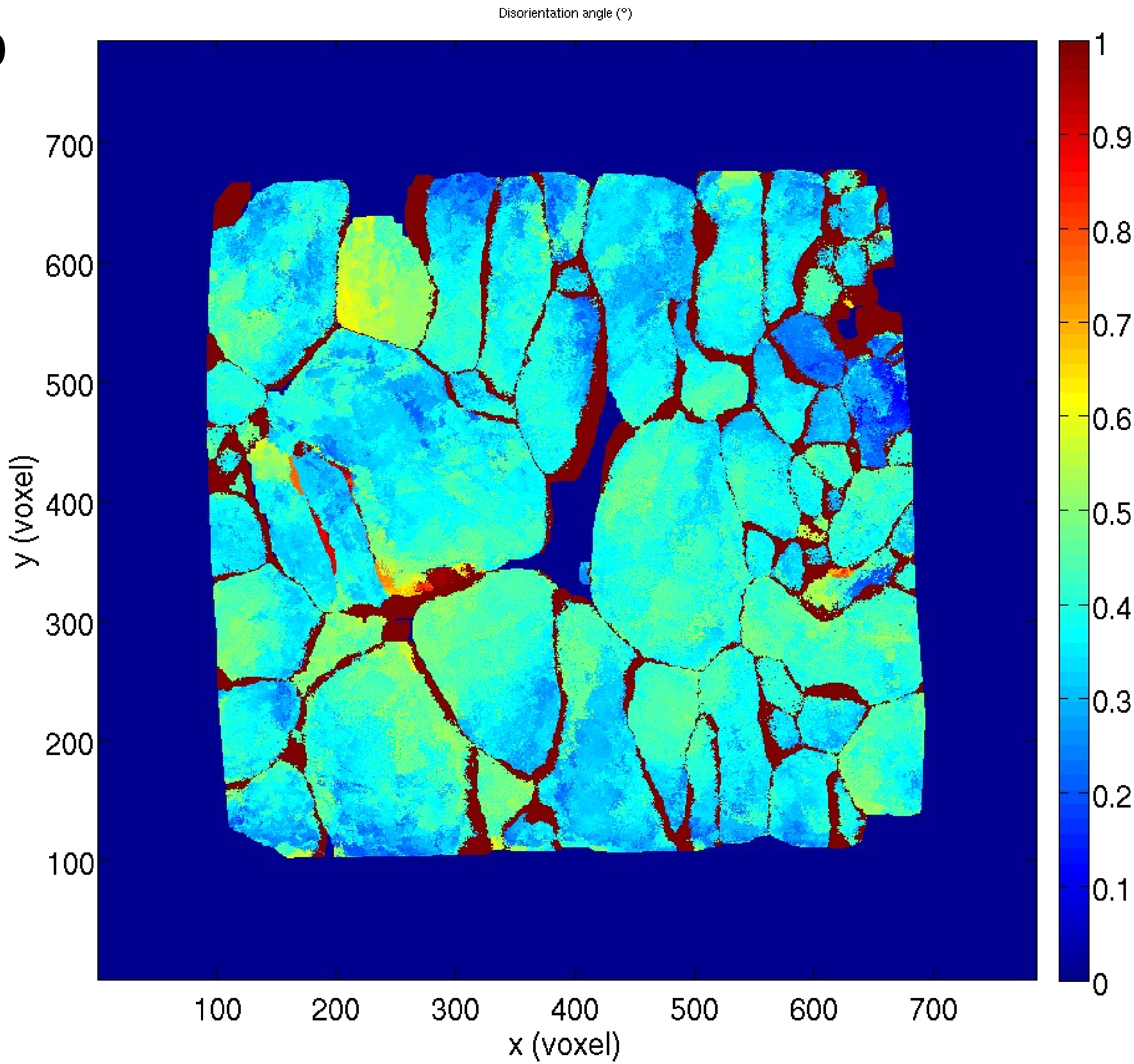
- Plastic deformation can result in an orientation change:

  If the deformation doesn't change the intrinsic structure of the coordinate system, it simply results in a rotation of the said system.



OK, but what about deformation in grains?

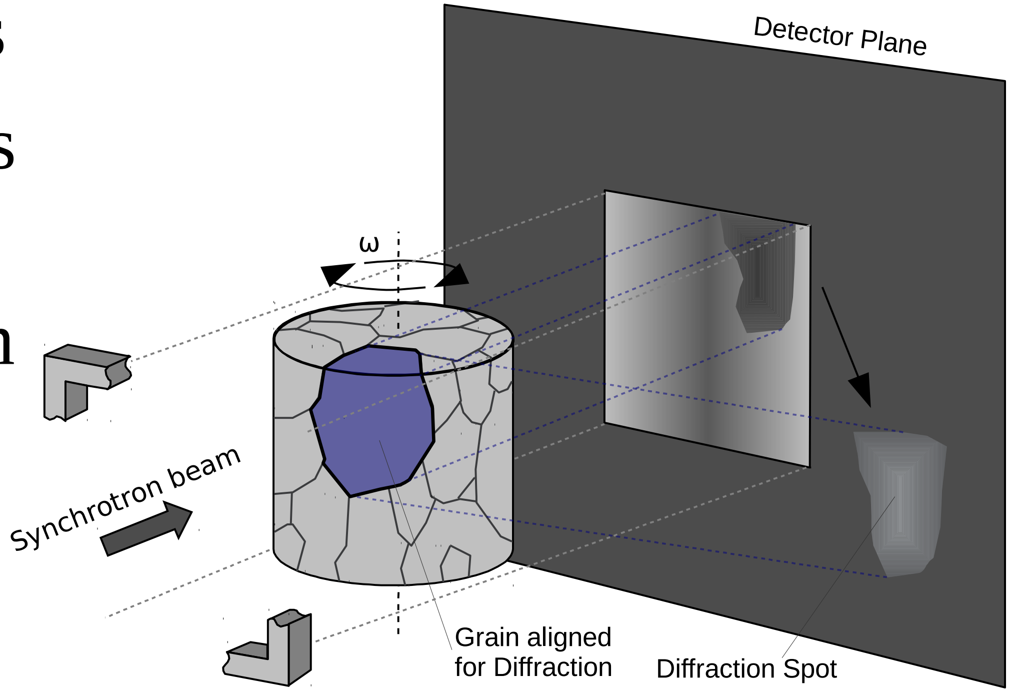
- Disorientation map for a poly-crystal:
- Highest levels of deformation at the grain boundaries.



Summary

- Introduction to Diffraction Contrast Tomography
- Materials with Deformation
- Our Model / Algorithm
- Results
- Conclusions

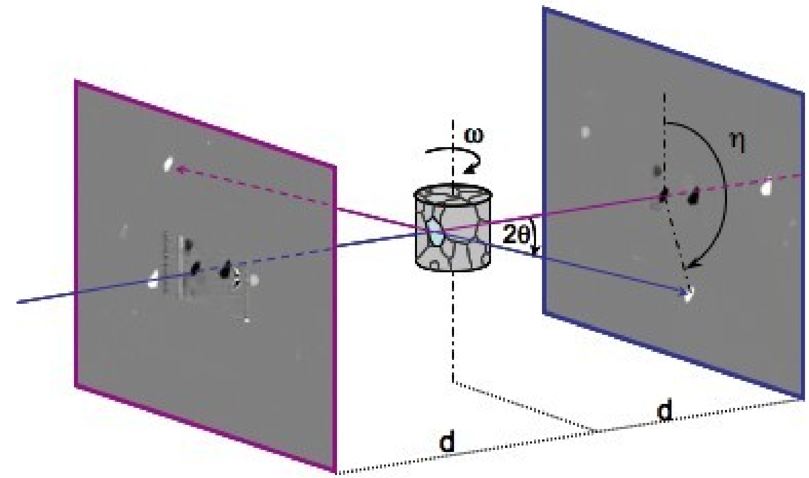
- Diffraction Contrast Tomography is a non-destructive characterization of 3D grain microstructure:
  - Assumes undeformed materials
  - Uses 2D monochromatic beams
  - Simultaneous acquisition of transmitted and diffracted beam
  - Acquisition time: 0.1-10h
  - Performs a continuous rotation over 360°, with steps of 0.05-0.1° (7200-3600 images)



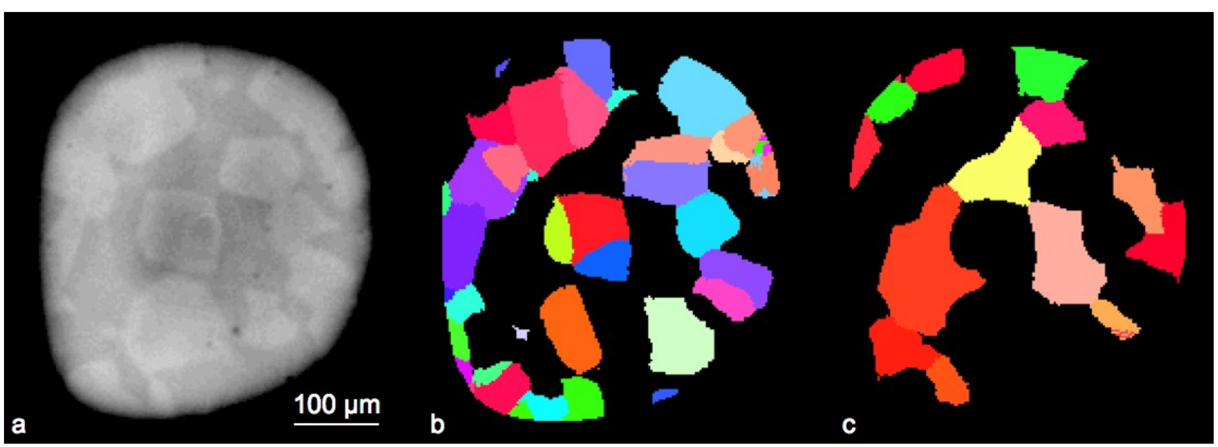
W. Ludwig et al., Rev. Sci. Instr. 2009

Intro to Diffraction Contrast Tomography 2/2

- Using the Friedel pairs it is possible to index the grains
- Diffraction spots as projections
- We use traditional oblique angles tomography codes to reconstruct the shape of the grains



- This also works for multi-phase materials!



a) Phase Contrast Tomography
b) DCT – Austenite
c) DCT – Ferrite

P. Reischig et al., J. of Applied Crystal 2013

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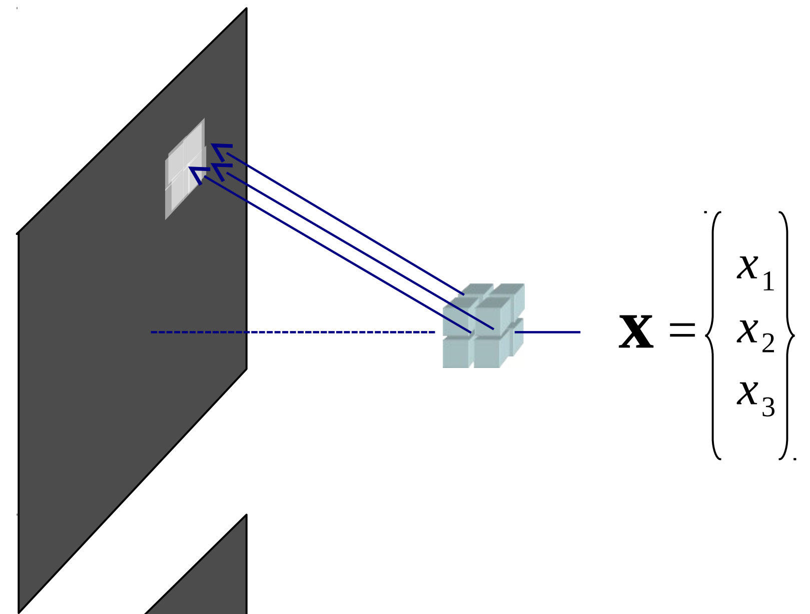
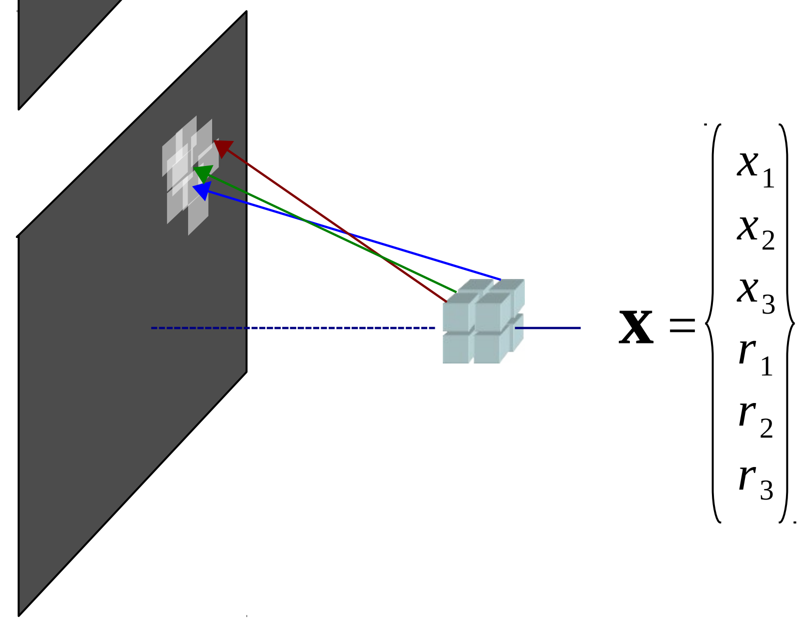
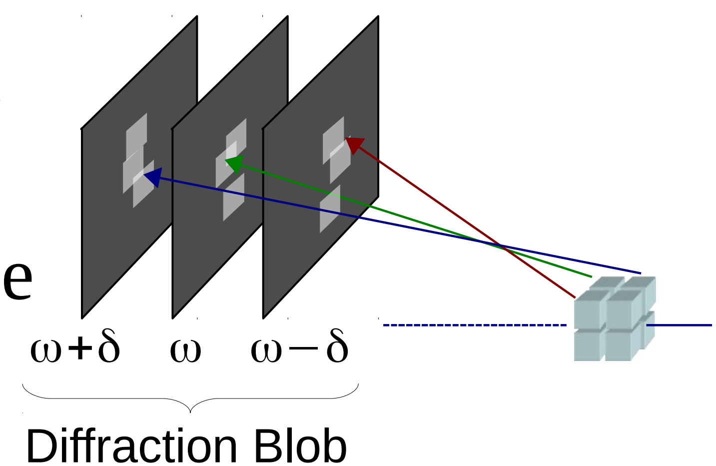
Reconstruction of (un)deformed material

- Given a 3D voxellated volume
  - If not deformed:
    - All voxels have same projection angle
    - Simple (line) back-projection geometry
    - Can be handled as a 3D (oblique angle) ART problem
  - If deformed:
    - Vector (Tensor) field with 3 (9) unknowns Or equivalently: scalar 6D (12D) problem
    - Complicated back-projection geometry
    - Needs another approach...





- Strain is a small perturbation compared to the plastic deformation of the crystal lattice. If we ignore it:
  - The reconstruction representation can be modelled either as a 3D vector field, or as a 6D scalar field
    - In the 3D vector field representation, each vector of each voxel is the associated local average orientation
    - In the 6D scalar field representation, each intensity of each voxel is the intensity of the “diffraction signal” for the given point of the extended representation
  - The deformed projection geometry both distorts the projected images, and spreads the signal over multiple images, for each projection



$$\mathbf{X} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ r_1 \\ r_2 \\ r_3 \end{pmatrix}$$

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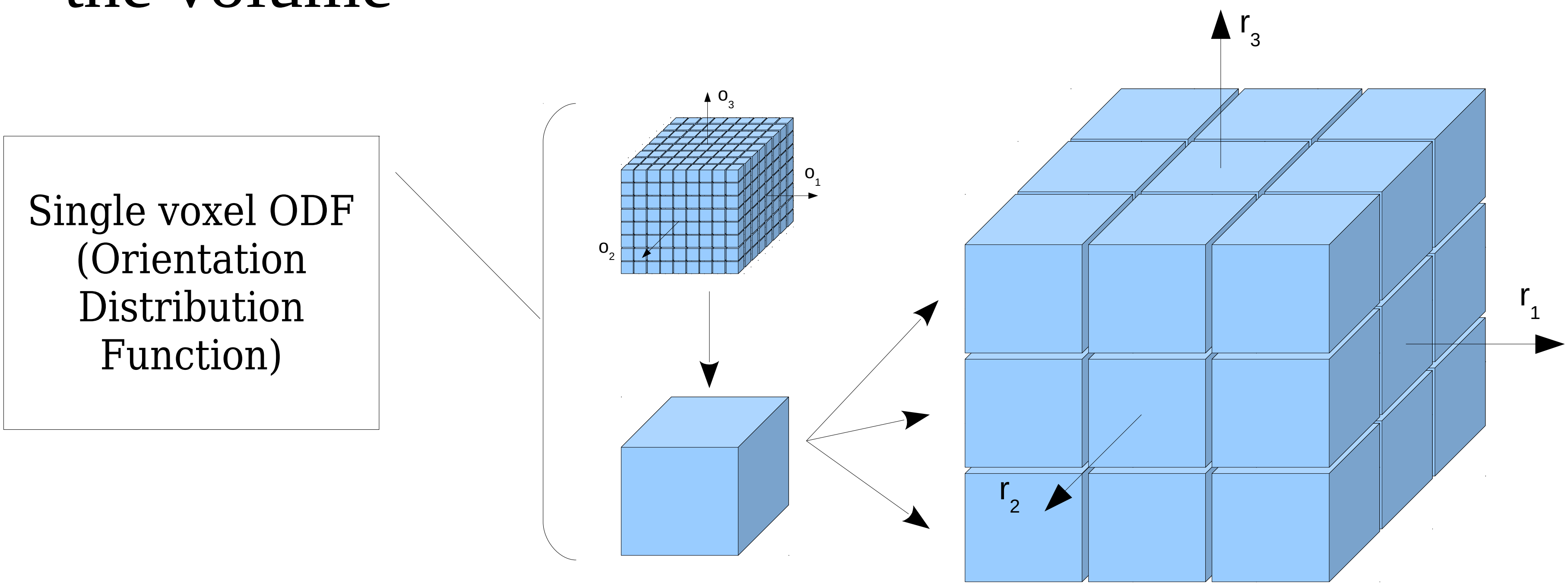
Insight of the 6D space

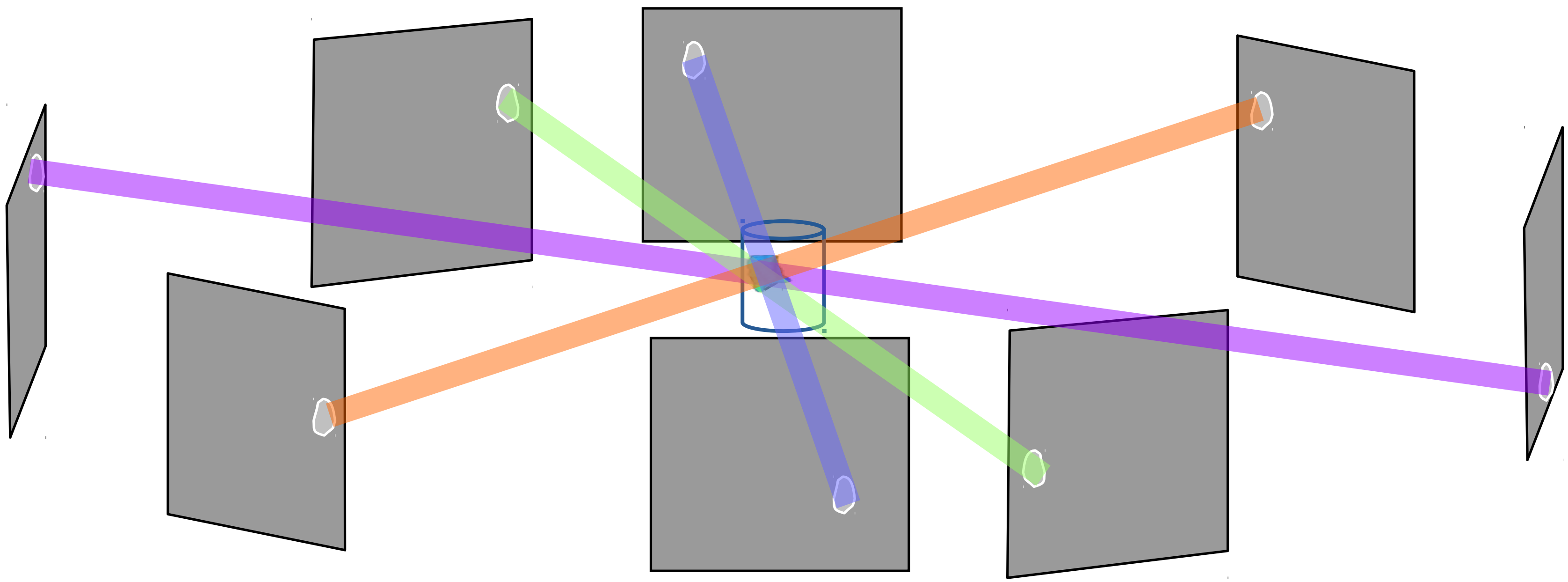
- 3D orientation-space volume that forms an ODF
- 3D real-space a collection of one ODF for each voxel in the volume



- In our implementation we do the inverse: 3D real-space volume are the voxels of a 3D orientation-space

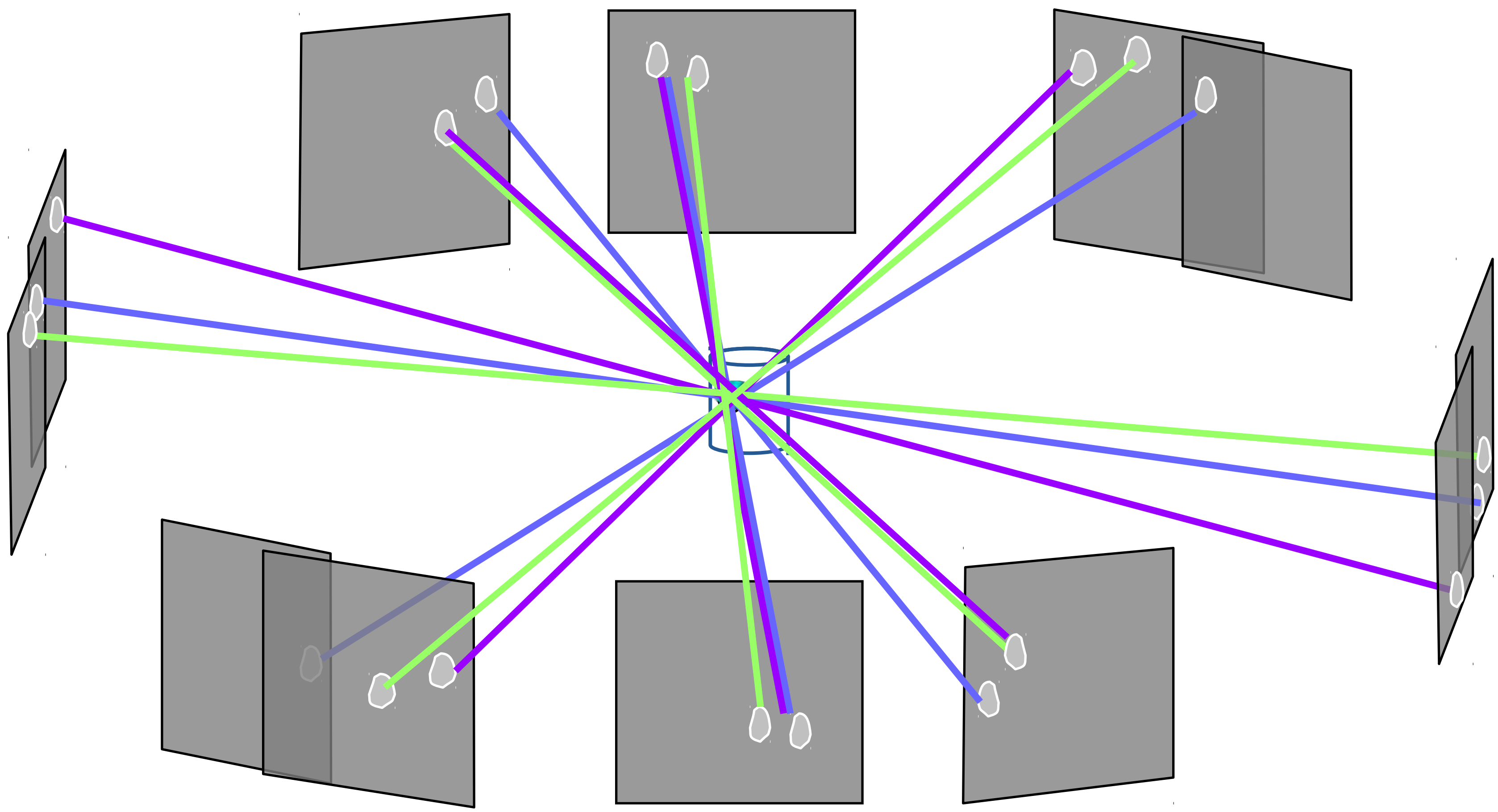
Projection geometry in standard DCT

- Undeformed grains will project to the same ωs



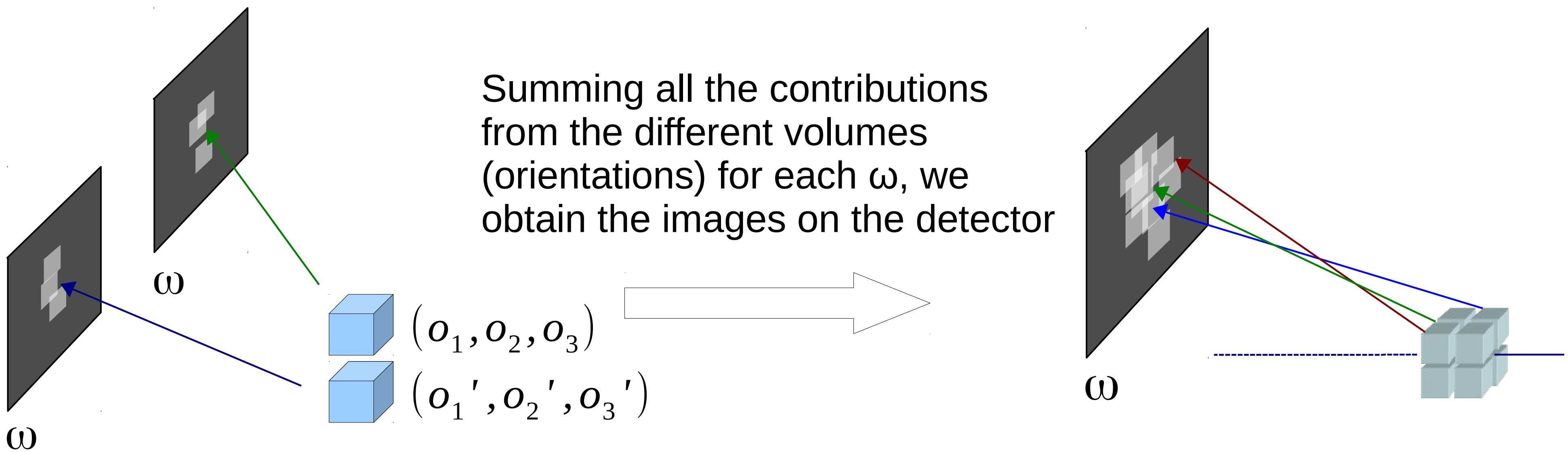
- Oblique angle reconstruction, using traditional algorithms (e.g. SIRT)

- Projection geometry of three different orientations:



- Tomography can be represented as: $W \underline{x} = \underline{y}$
- To deal with indeterminacy and noise: $\min \varphi(\underline{x}) = \|W \underline{x} - \underline{y}\|_2^2$
- Our case is not so "easy": $W_{(\underline{x})} \underline{x} = \underline{y}$
- But we linearised it! (by unfolding-sampling the 6D space, at the expense of multiplying the unknowns)
- Assuming that only few of these orientations will be active in each real-space voxel, we can look for a sparse solution (l1-min): $\min \varphi(\underline{x}) = \|W \underline{x} - \underline{y}\|_2^2 + \lambda \|\underline{x}\|_1 \quad s.t.: \quad \underline{x} \geq \underline{0}$
- Or, if the density is homogeneous in the grains, we could apply a "flatness" constrain on the 3D space representation: $\min \varphi(\underline{x}) = \|W \underline{x} - \underline{y}\|_2^2 + \lambda\, TV(S \underline{x}) \quad s.t.: \quad \underline{x} \geq \underline{0}$

- The implementation is pretty simple: there's a $1 \leftrightarrow 1$ relationship between the mathematical objects and the functions of the algorithm:
  - W is the projection of all the volumes to the detector



  - W^T is the back-projection of the images on the detector to the volumes

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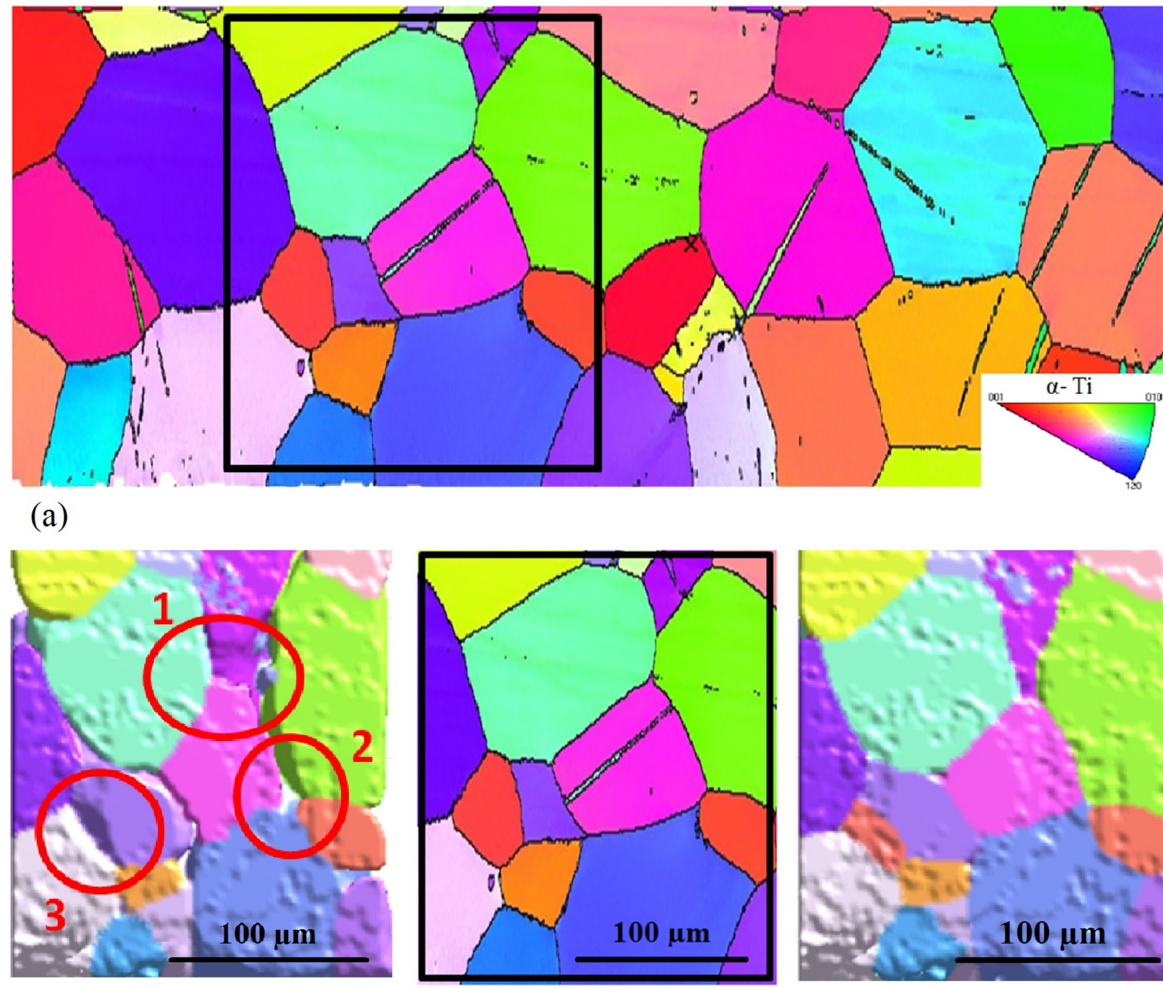
- Comparing a reconstruction using the 3D-DCT and 6D-DCT on the surface sensitivity, against EBSD measurements

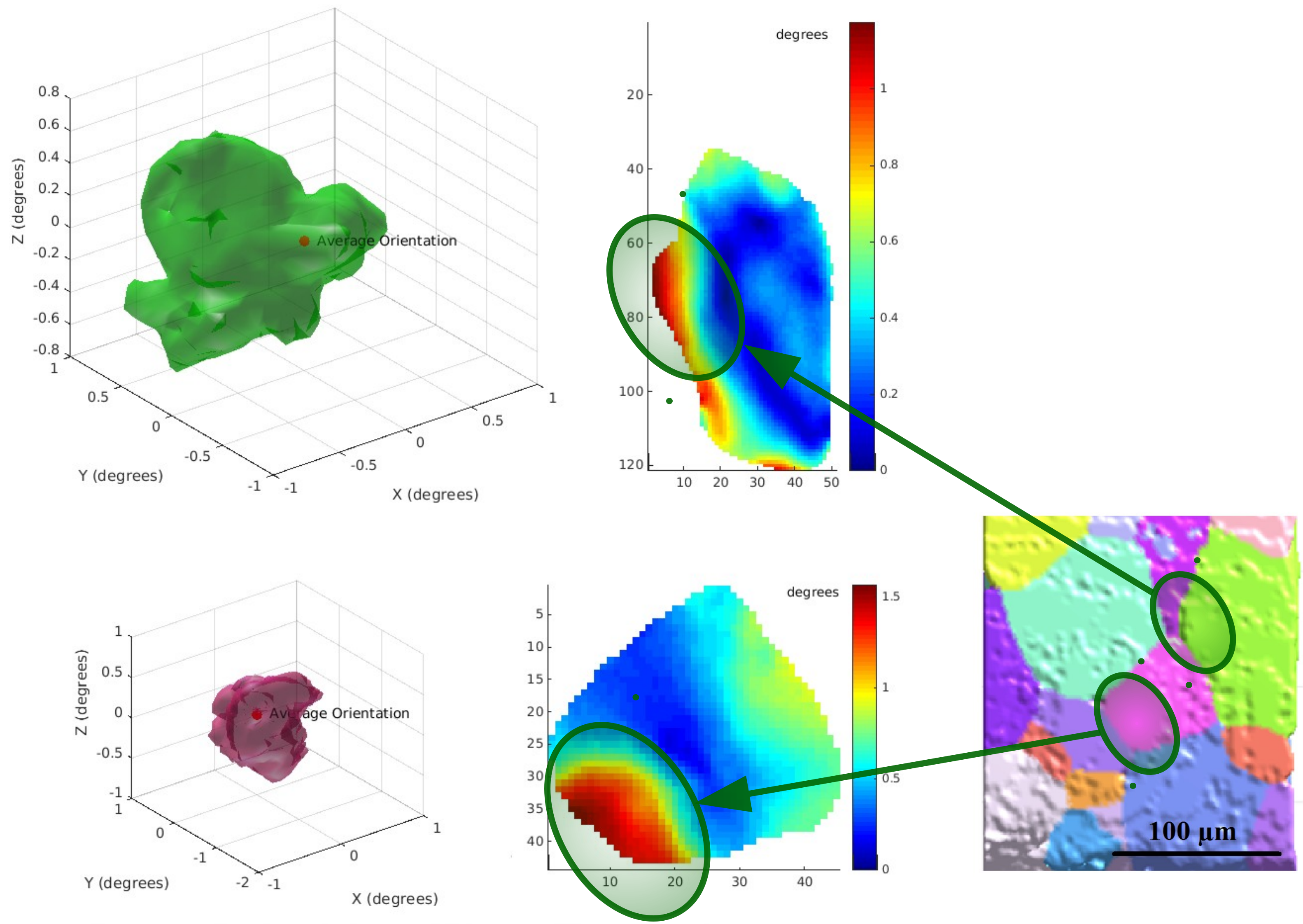
(a) EBSD – Full surface
(b) 3D-DCT – ROI
(c) EBSD – ROI
(d) 6D-DCT – ROI



(a) (b) (c) (d)

Deformation in Ti sample

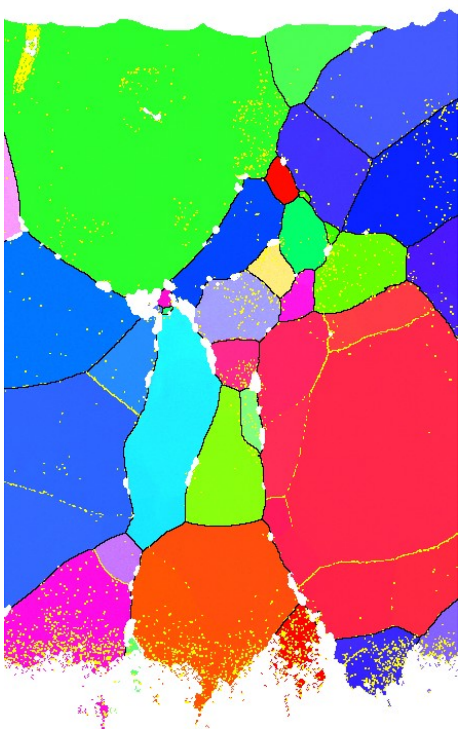
- Looking at the reconstructed deformation:



NaCl sample (up to 1-2 deg of deformation)

- Surface:

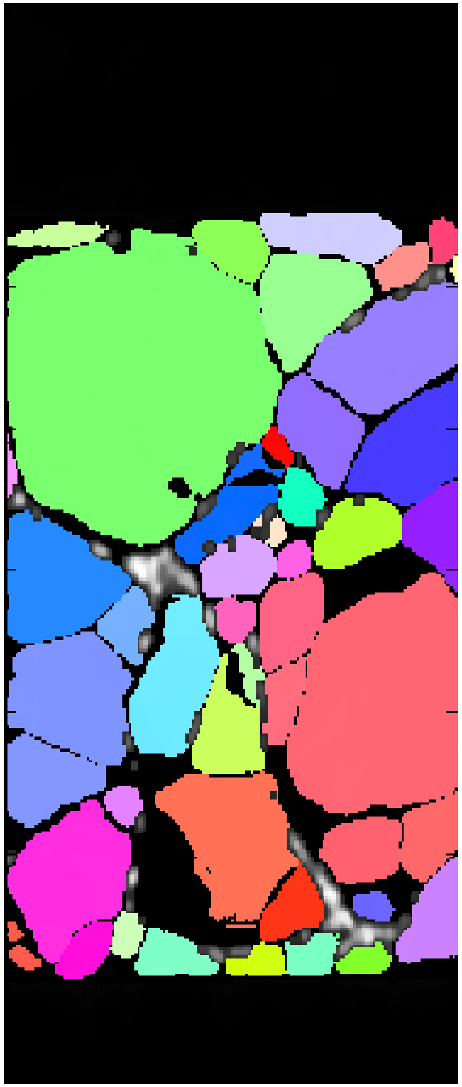
(1) Each indexed grain alone
(2) With clustering and extension



EBSD

3D-DCT

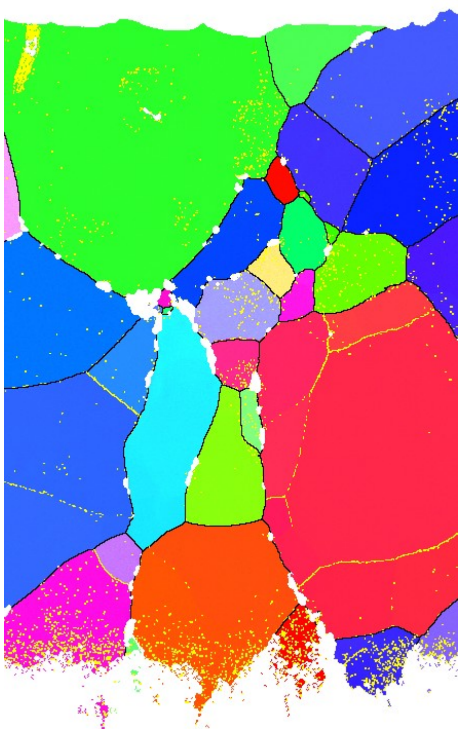
6D-DCT



Real Data (up to 1-2 deg spread)

- Surface:

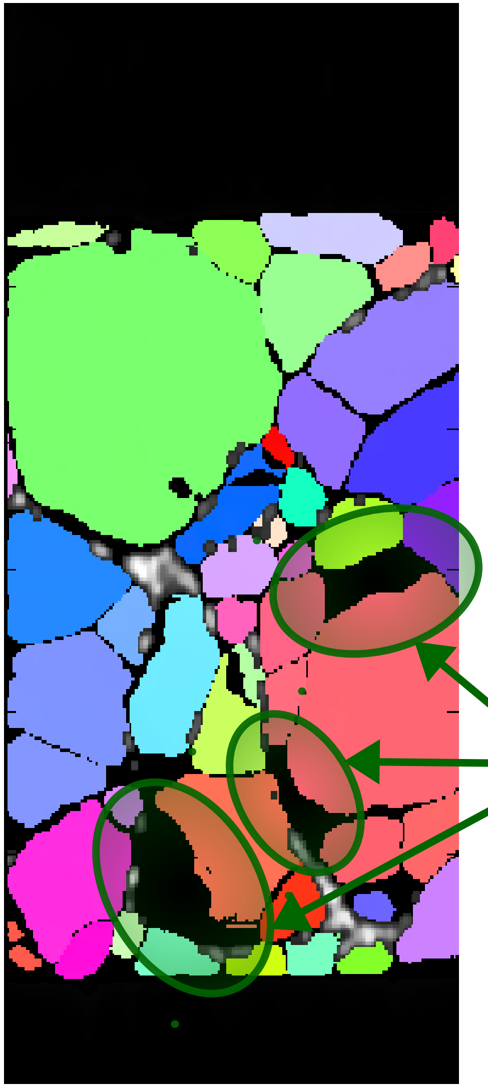
(1) Each indexed grain alone
(2) With clustering and extension



EBSD

3D-DCT

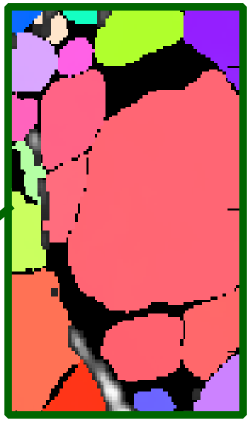
6D-DCT

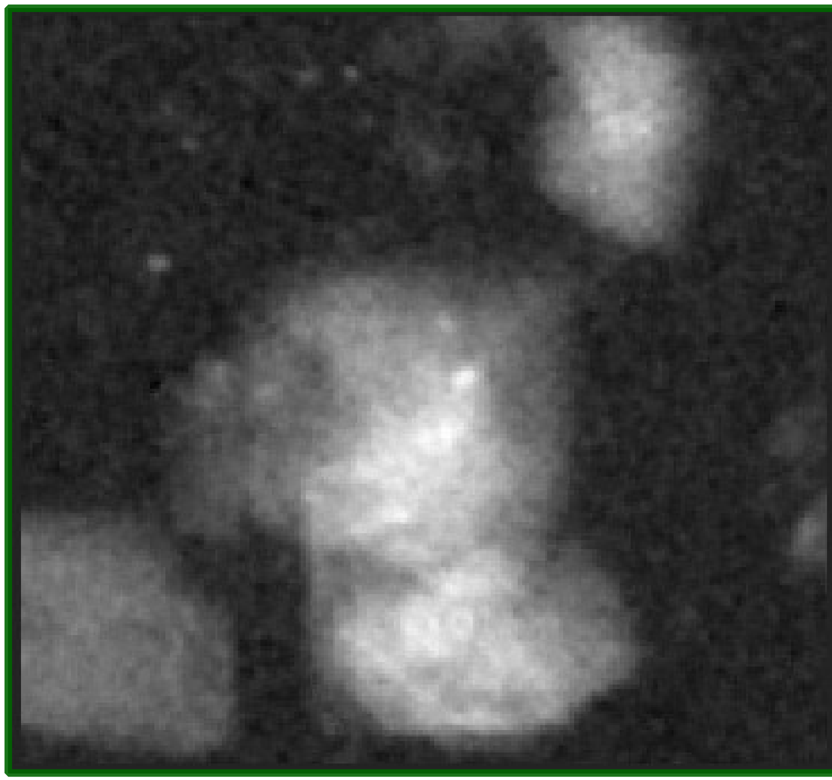


Why are those regions missing, and what can we do about it?

Cluster reconstructions 1/2

- Can we use the 6D algorithm to index grains?
  - What if we simply tried reconstructing from the raw detector images taken from an arbitrary bounding box in the 6D-space?
  - Let's use the indexed grains from a cluster to define the 6D bounding box:

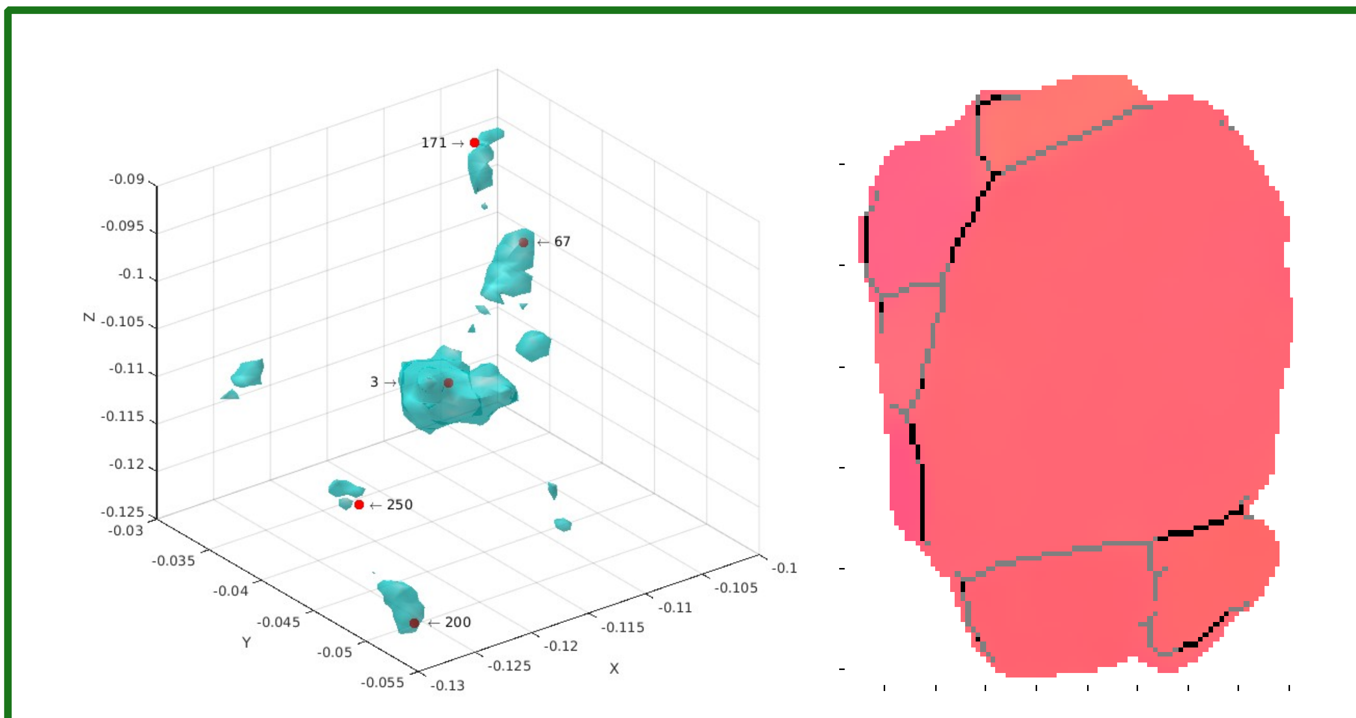




Sum of all the omegas from one of the blobs defined by the 6D bounding box, when projected to the detector

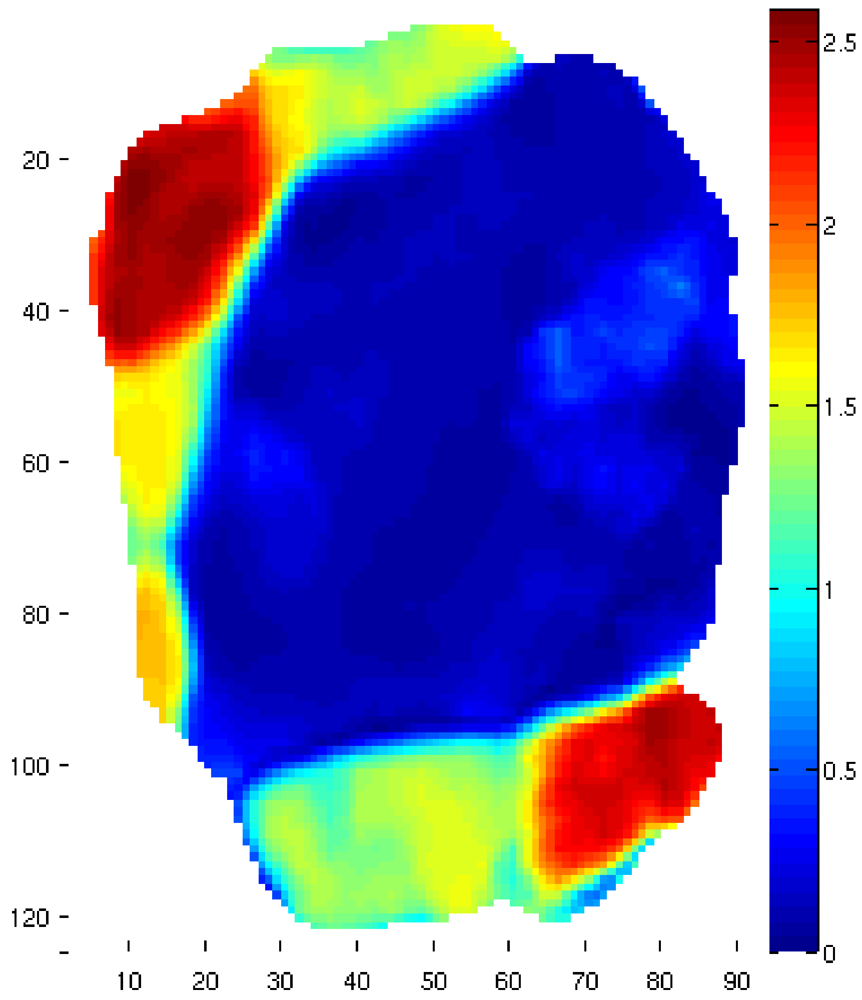
A [2 2 2] reflection at:
$\theta = 6.21°$
$\eta = 112.112°$
$\Delta\omega = 6.7°$ (67 images)

- Can we use the 6D algorithm to index grains?
  - What if we simply tried reconstructing from the raw detector images taken from an arbitrary bounding box in the 6D-space?
  - Let's use the indexed grains from a cluster to define the 6D bounding box:



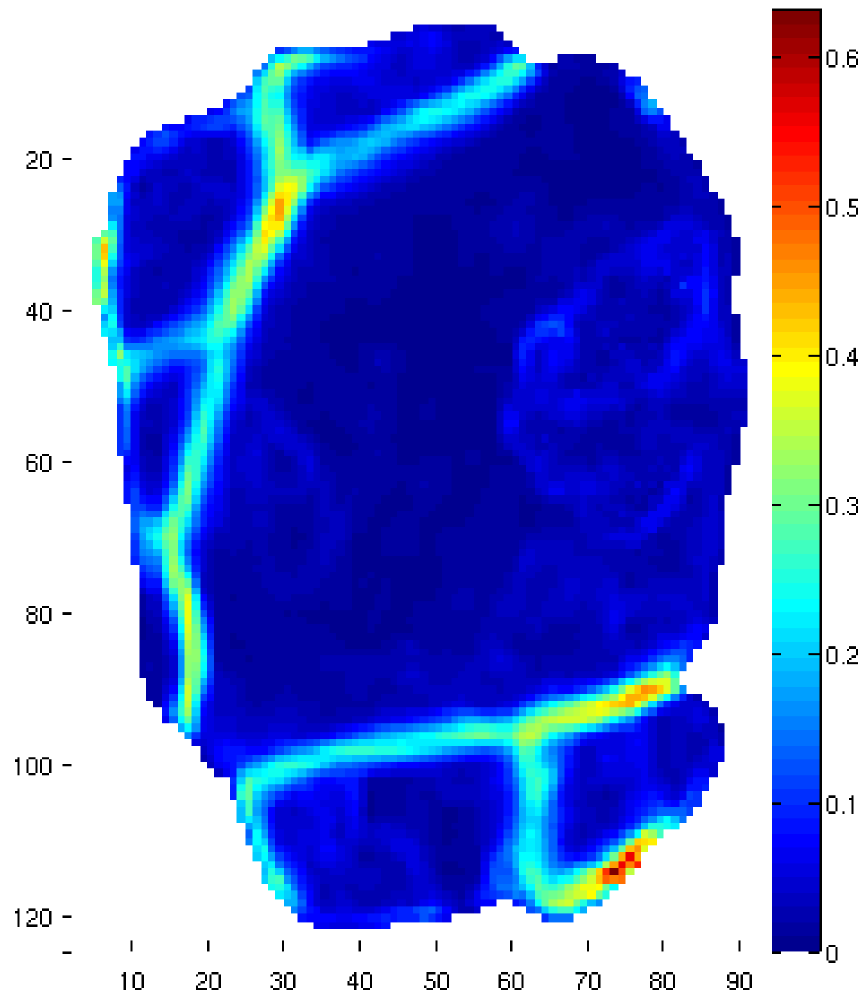
IGM

Intra-Granular Misorientation



KAM

Kernel Average Misorientation



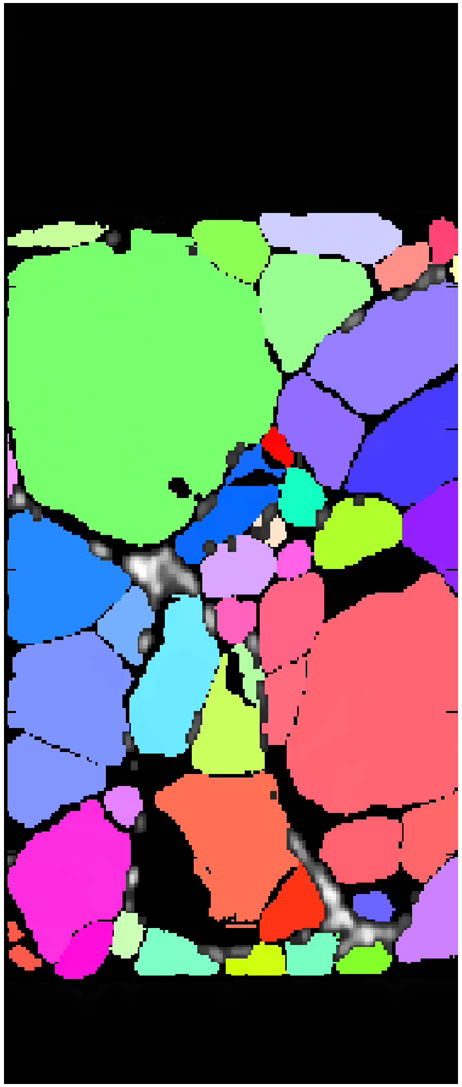
Real Data (up to 1-2 deg spread)

- Surface:

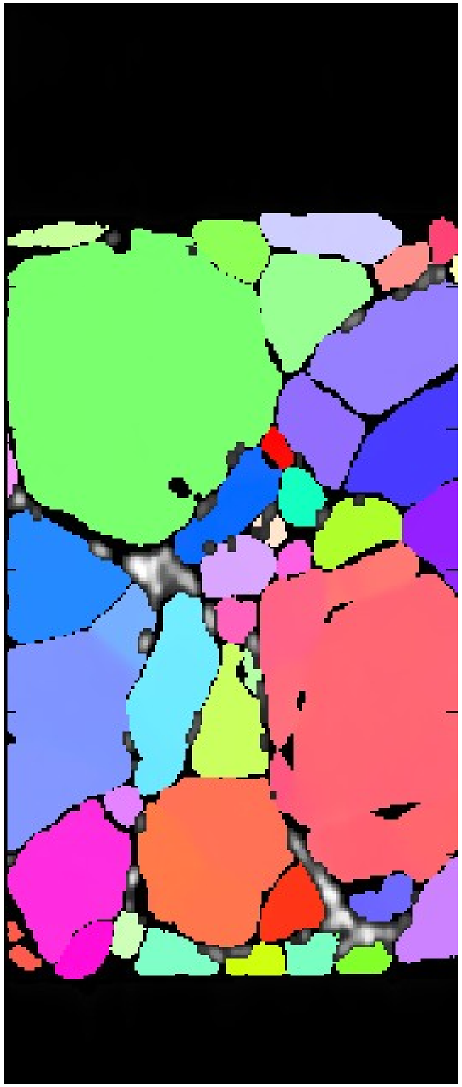
(1) Each indexed grain alone
(2) With clustering and extension

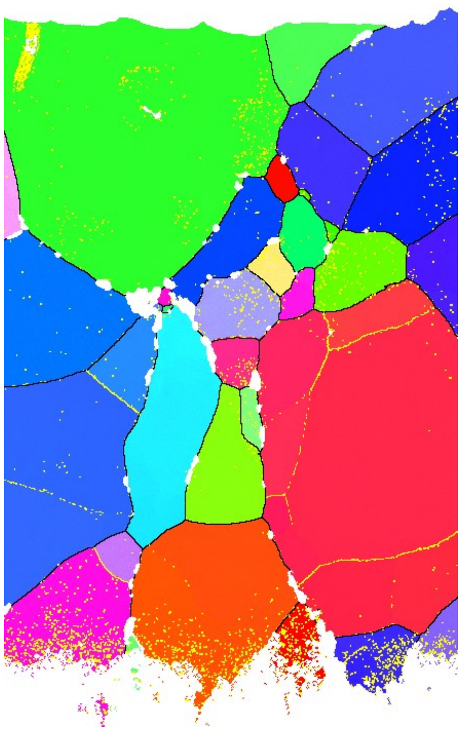
3D-DCT

6D-DCT[1]



6D-DCT[2]





EBSD

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Recap of the main ideas

- In this model we represent each voxel as a stack of discretized orientations, each representing the contribution of that voxel to a particular orientation.
- Allowing many orientations per each voxel, it blows up the number of unknowns
- By minimizing the l1-norm of the 6D representation, sparse solutions are prioritized, thereby improving the ability to reconstruct using far more unknowns than equations
- Sampling in the orientation domain is an essential topic

Conclusions

- Real data shows very good improvements especially for those scenarios (surface sensitivity) where traditional DCT had more troubles.
- Can complement indexing techniques
- Shows potential for further improvements and extensions:
  - Use of Far-field information
  - Overcome spot/blob segmentation issues
  - Overcome overlap on experimental images