UNIVERSITY OF CAMBRIDGE

3D Neo-Eulerian Misorientation Spaces

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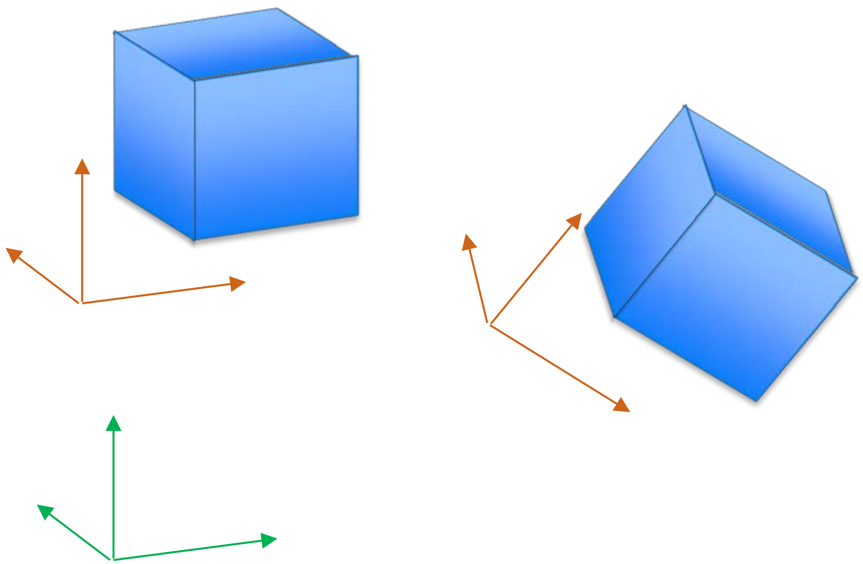
Content

Introduction

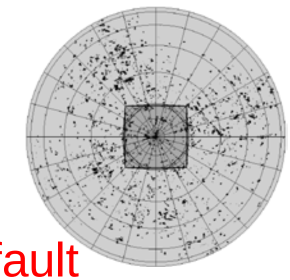
- Materials and rocks often contain multiple crystals (polycrystalline)
  - Ori. and Misori. are critical to both materials science and earth sciences
- Crystallographic mapping techniques contain a wealth of data
  - Often under-utilised, 3D data must be analysed in 3D spaces



3 Euler angle: $\phi1$, Φ, $\phi2$

Matrix: 3 columns

Axis-angle: 3D vector **n** x f(ω)



Axis-angle space default

=

Sphere with radius ω = 180 degree

Introduction

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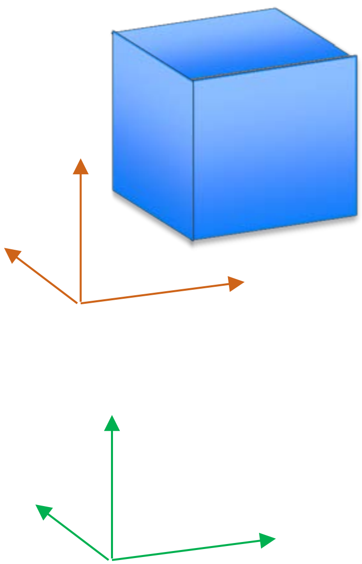
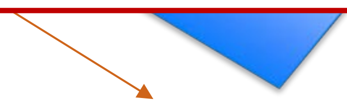
  - Ori. and Misori. are critical to both materials science and earth sciences
- Crystallographic mapping techniques contain a wealth of data
  - Often under-utilised, 3D data must be analysed in 3D spaces

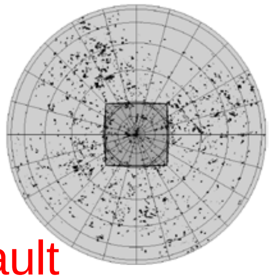
- Orientations and Misorientations are defined by 3 independent variables
- Orientations can be treated like a special case of Misorientations (triclinic)
- 3D data should be plotted in 3D spaces (except very good reasons)

Φ, $\phi 2$

ctor **n** x f(ω)







Axis-angle space default

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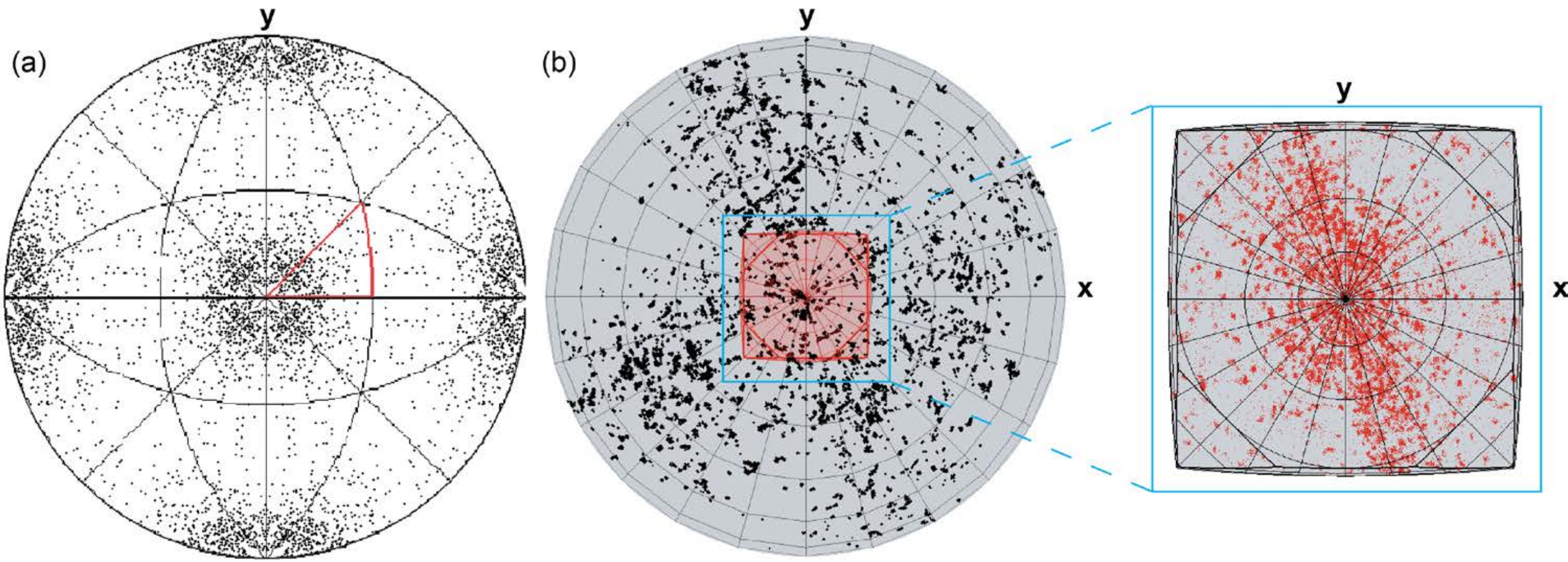
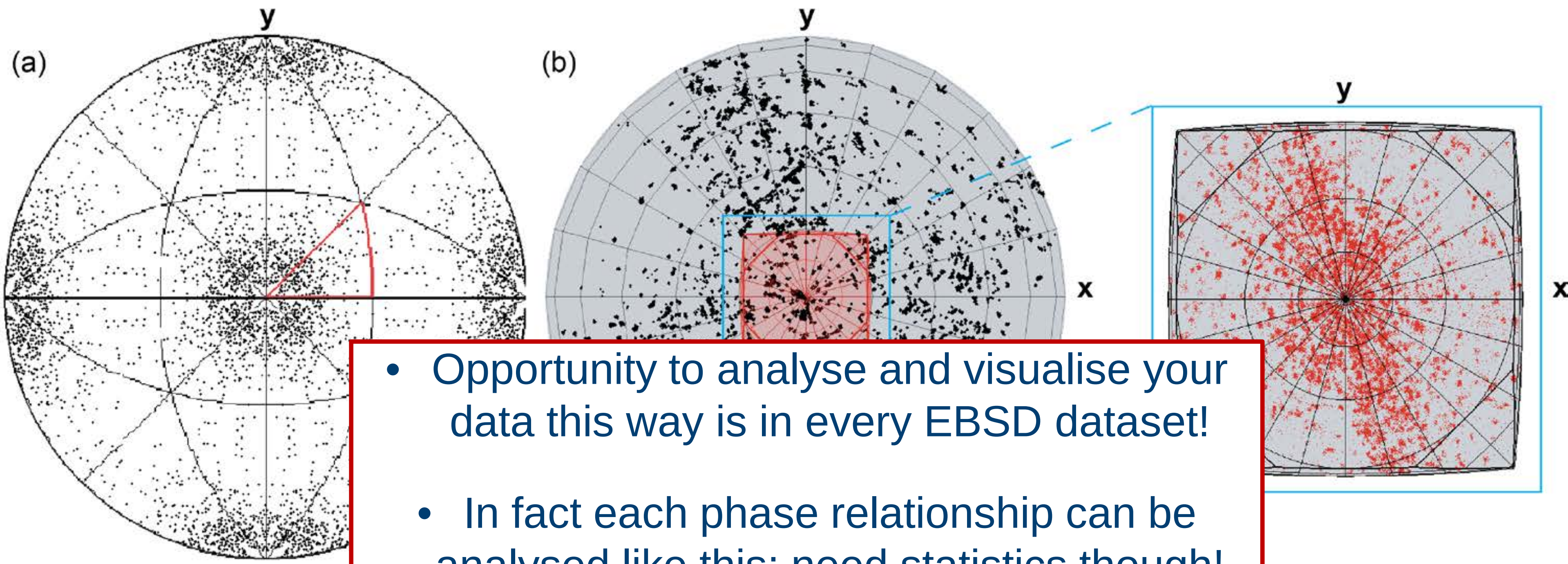
Sphere with radius ω = 180 degree

Example of cubic Symmetry (m-3m)



- Example FundamentalZone = domain of disorientations
- Each symmetrically equivalent misorientation is contained only once

Example of cubic Symmetry (m-3m)

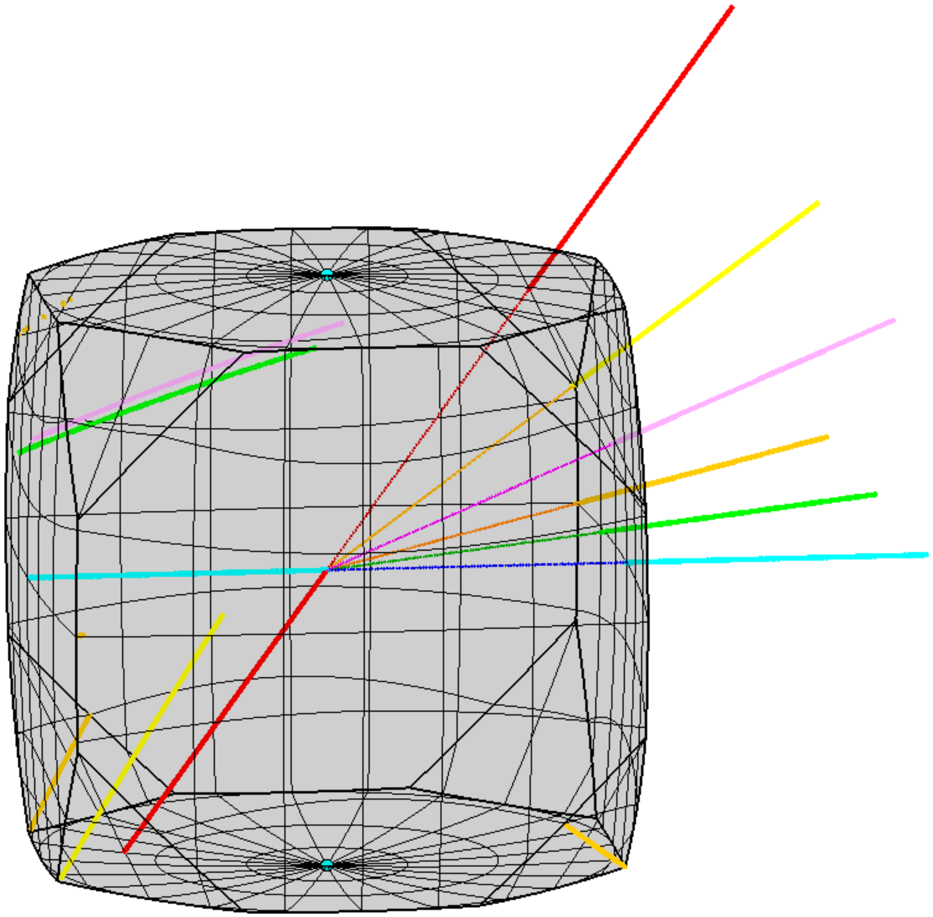


- Opportunity to analyse and visualise your data this way is in every EBSD dataset!
- In fact each phase relationship can be analysed like this; need statistics though!

- Example FundamentalZone = domain of disorientations
- Each symmetrically equivalent misorientation is contained only once

Properties of Fundamental Zones

- Symmetry operators: e.g. cubic $m\bar{3}m$ has 48, triclinic $\bar{1}$ has 2
- The higher the combined symmetry, the smaller the fundamental zone
  - FZs can be used as reference frames
- Aboriginal points and "umklapp" behaviour



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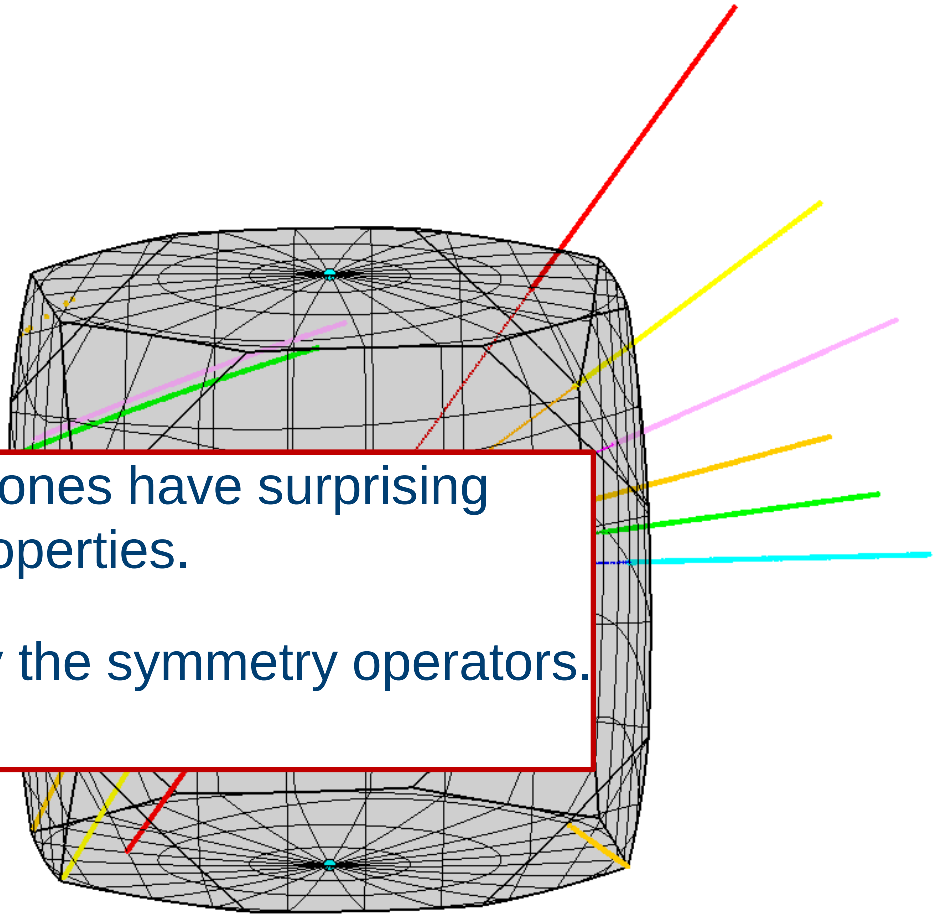
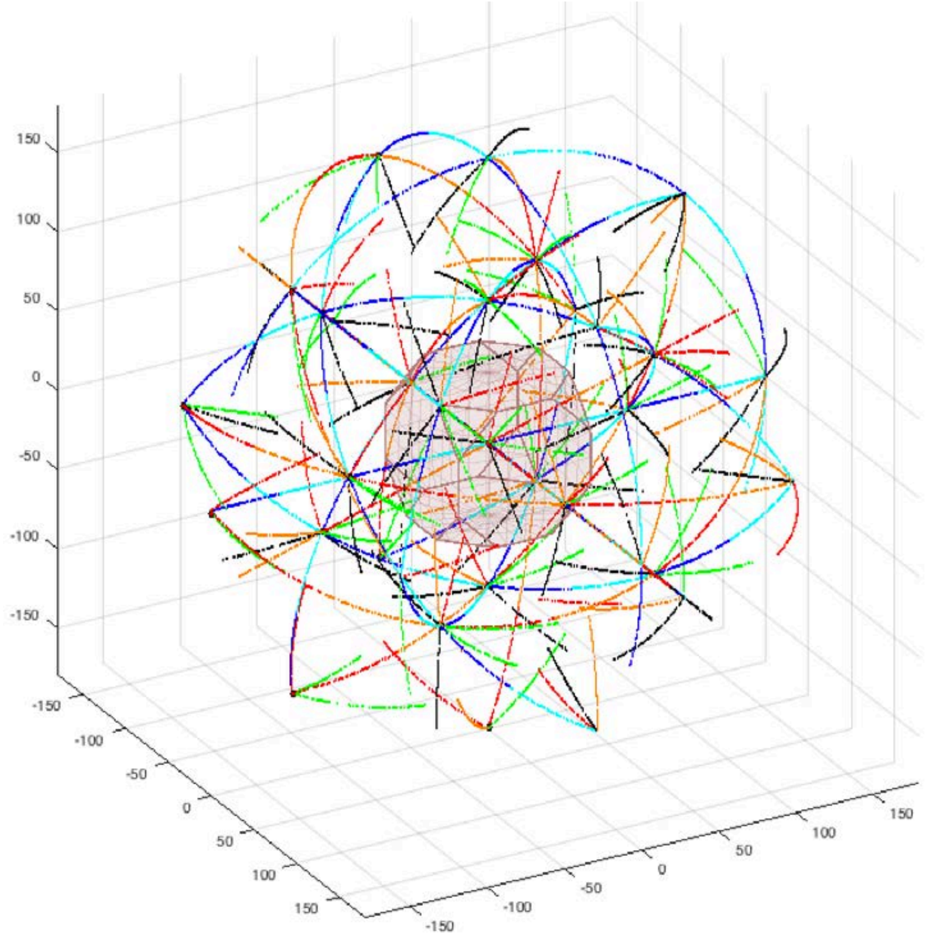
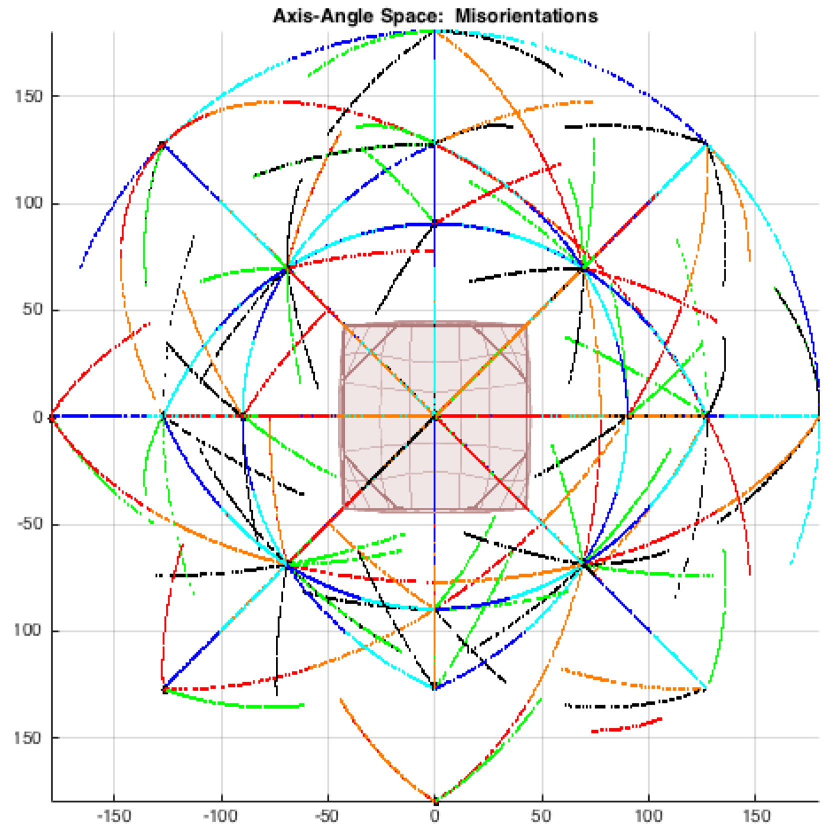


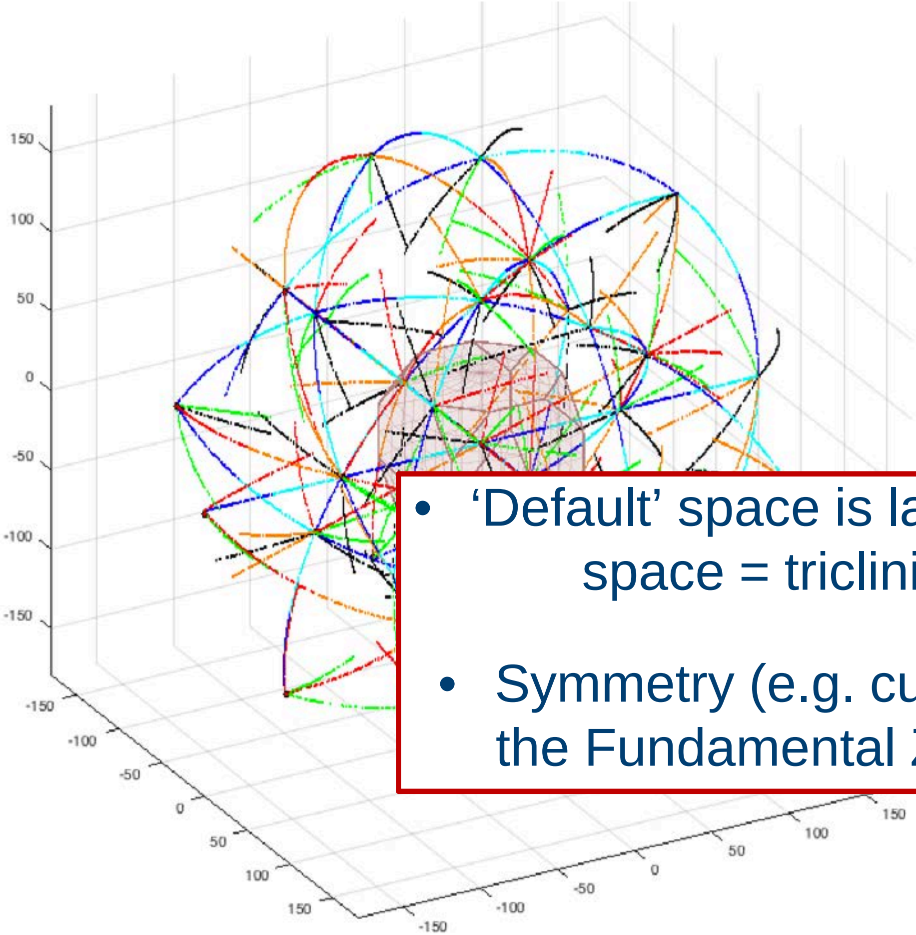
- Fundamental Zones have surprising properties.
- They are caused by the symmetry operators.

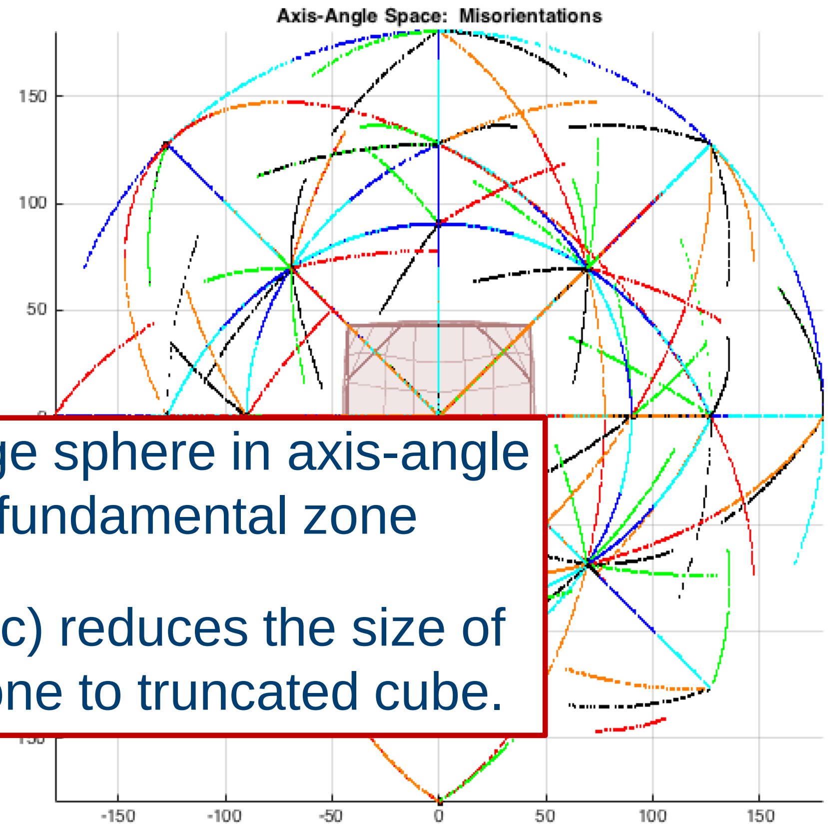
Properties of Fundamental Zones





Properties of Fundamental Zones





- ‘Default’ space is large sphere in axis-angle space = triclinic fundamental zone
- Symmetry (e.g. cubic) reduces the size of the Fundamental Zone to truncated cube.

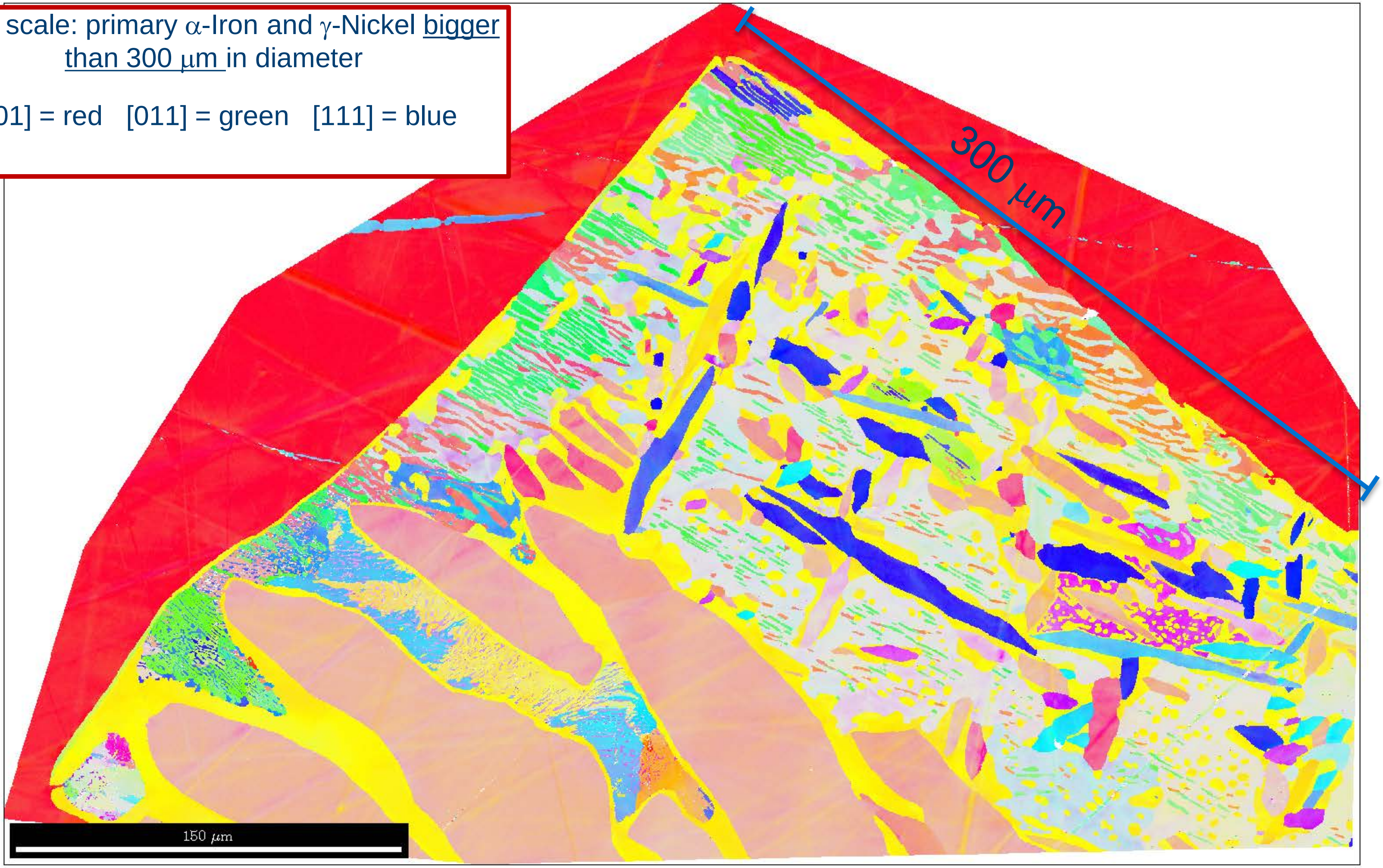
Example 1: Meteorite

Josh Einsle, Claire Nichols, Richard Harrison

- Formed 2 Ma after the solar system;
  - Break-up of the parent body occurred 450-750 Ma before now = 4.5 Ba old → way to Earth
- Mainly composed of Fe (α)-kamacite and Ni (γ)-taenite
- Classification: IAB parent body,
  Odessa (USA) – main group and
  Toluca (Xiquipilco, Mexico) – s(sub)LL(low gold, low nickel)
- Here: Odessa sample (ID 11538), borrowed from the Sedgwick Museum, Cambridge UK

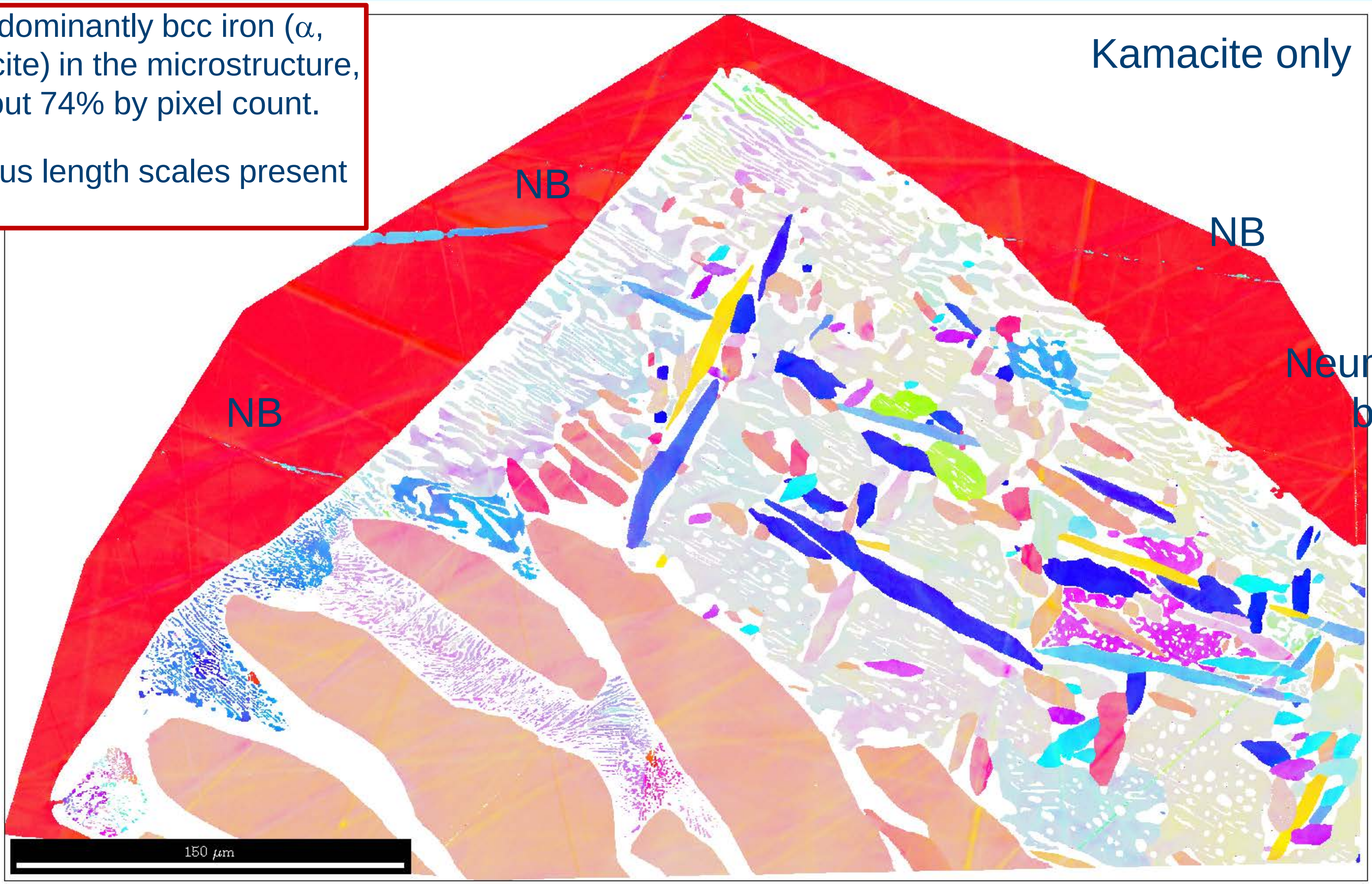
Full dataset: bcc Iron (α) and fcc Nickel (γ)

- Large scale: primary α-Iron and γ-Nickel bigger than 300 μm in diameter
  - [001] = red [011] = green [111] = blue



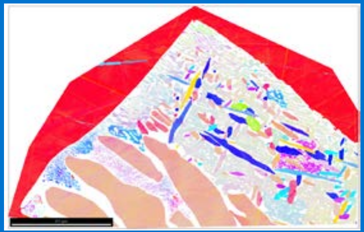
α-Iron (bcc) – Orientation Map

- Predominantly bcc iron (α, kamacite) in the microstructure, about 74% by pixel count.
- Various length scales present



NB = Neumann bands

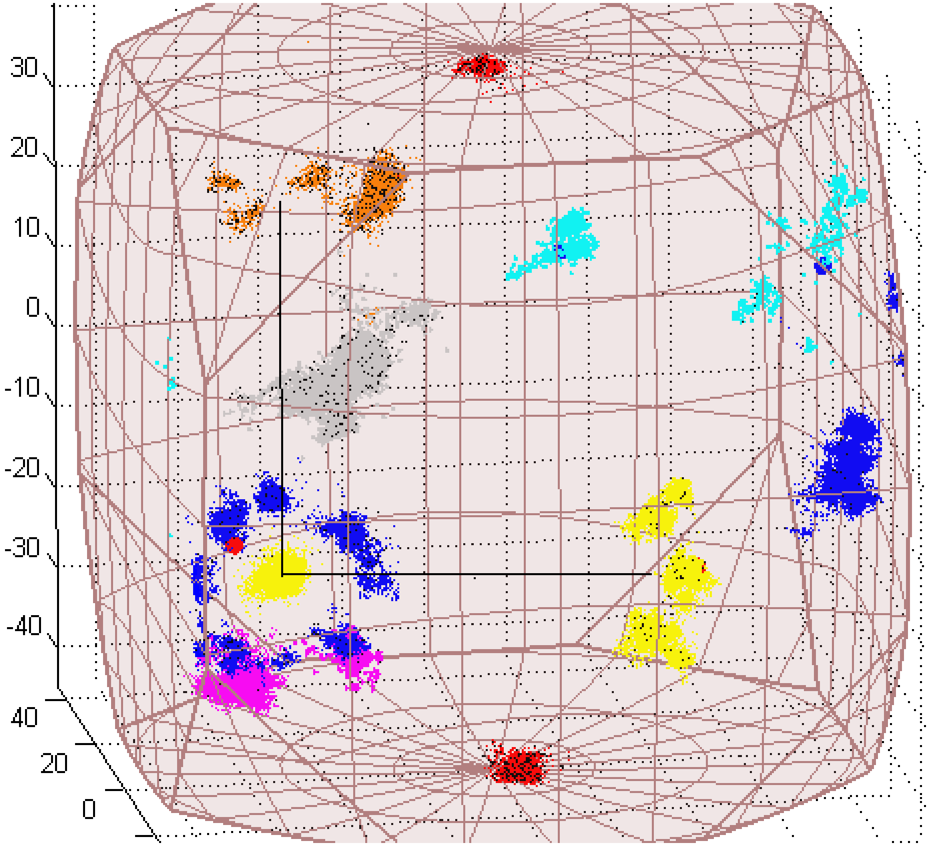
α-Iron (bcc) – Orientation Space (raw data)



Types of clusters

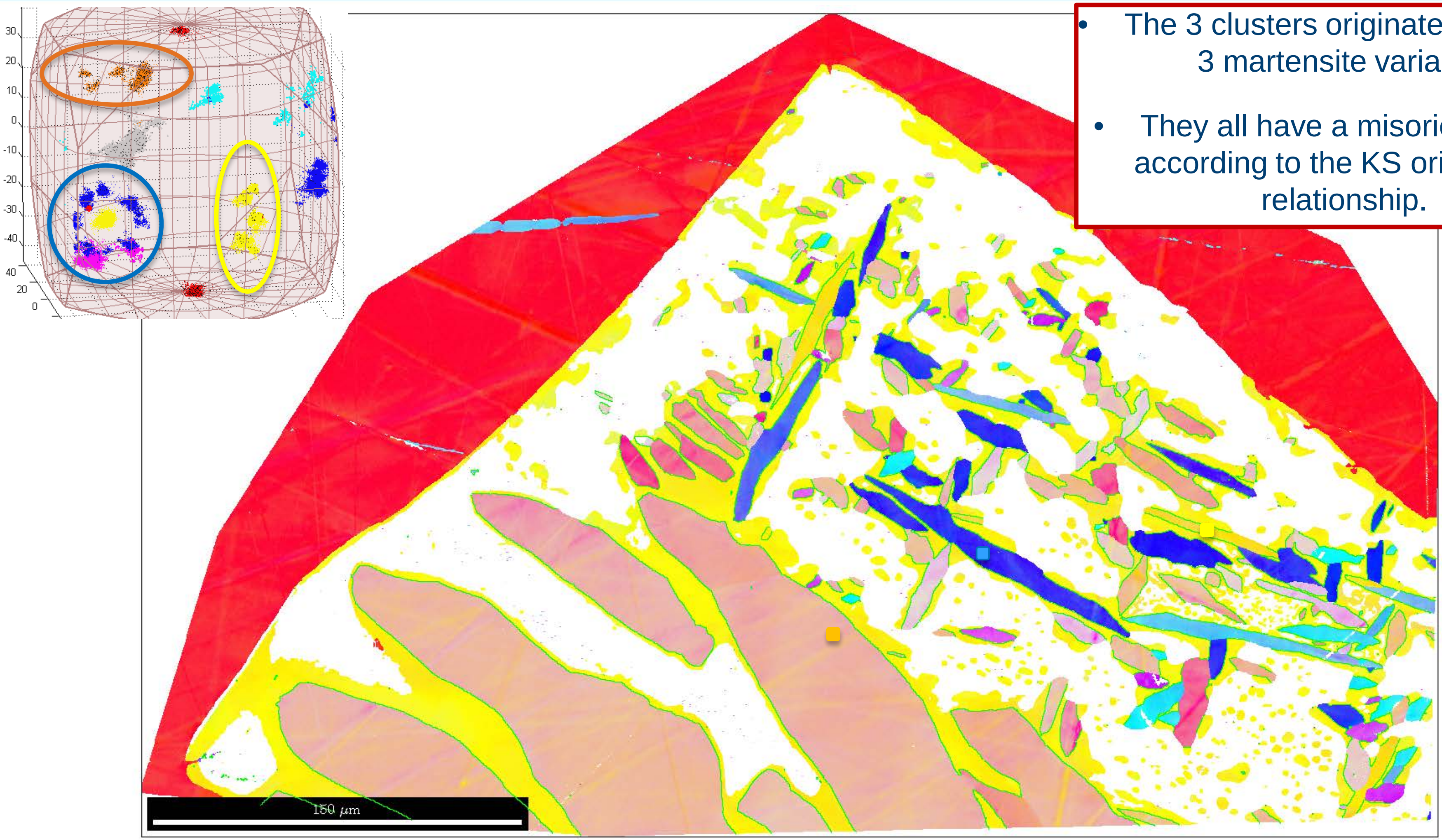
- Type 1: clear centre
- Type 2: ring-shaped

- There are 3 ring-shaped clusters, each centrosymmetric around a different axis.
- They are in a KS-type configuration with the parent austenite grain.



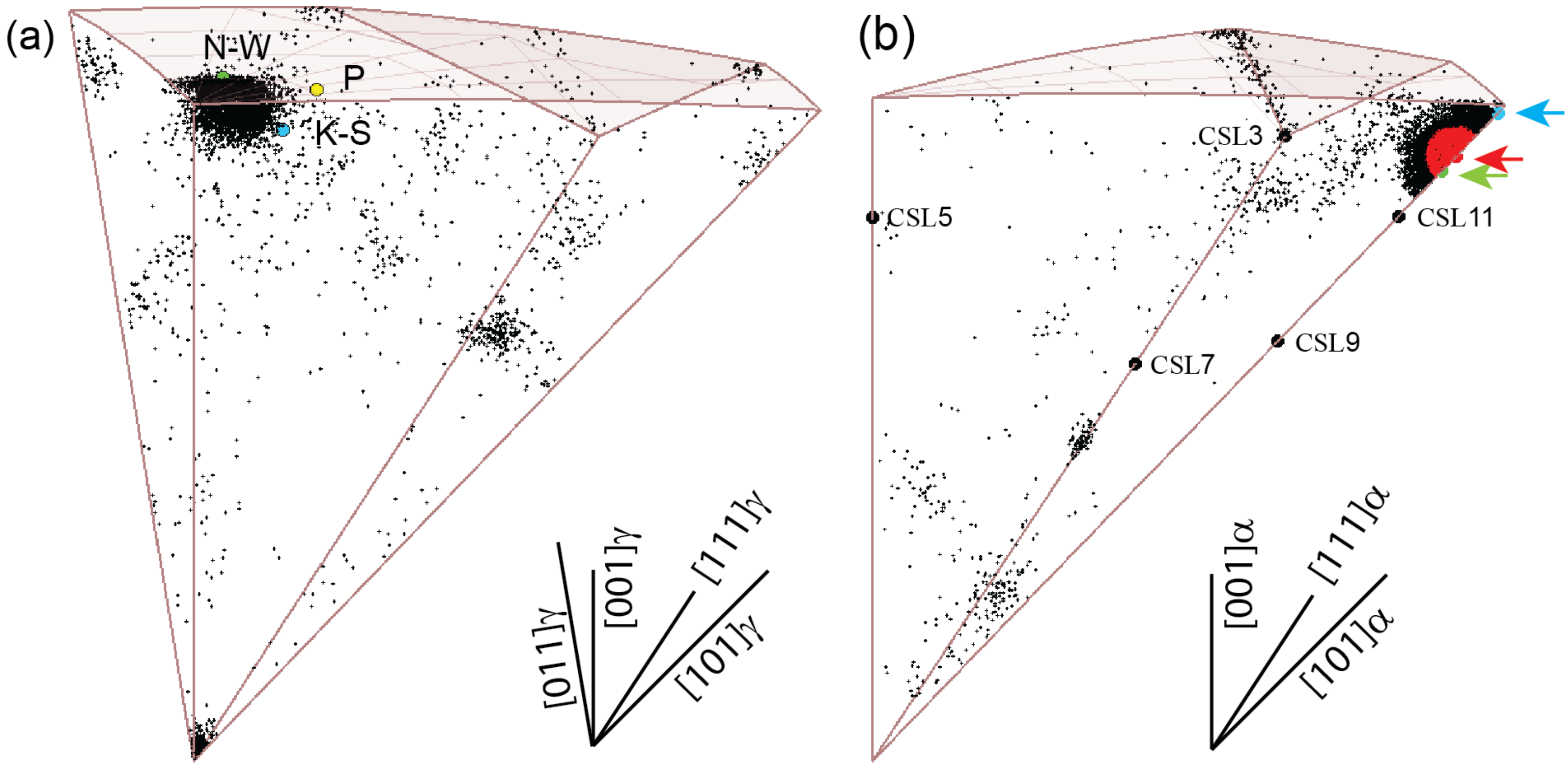

```
KS =
orientation('map',Miller(1,1,1,cs_aust),Miller(0,1,1,cs_ferr),...
  Miller(-1,0,1,cs_aust,'uvw'),Miller(-1,-1,1,cs_ferr,'uvw'));
```

Data selected: primary grains + 3 ring clusters

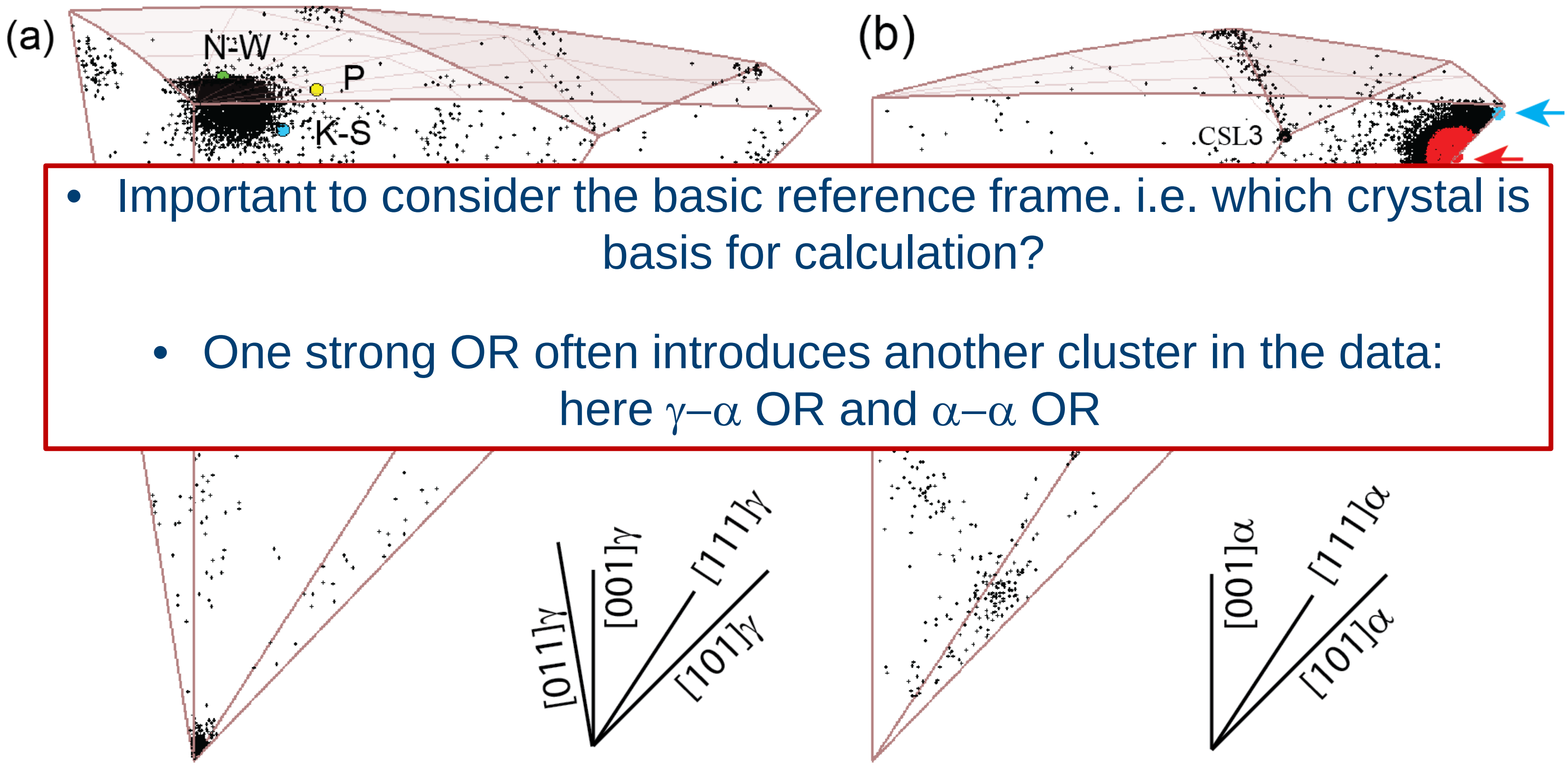


- The 3 clusters originate from the 3 martensite variants.
- They all have a misorientation according to the KS orientation relationship.

Similar example: bainitic steel



Similar example: bainitic steel

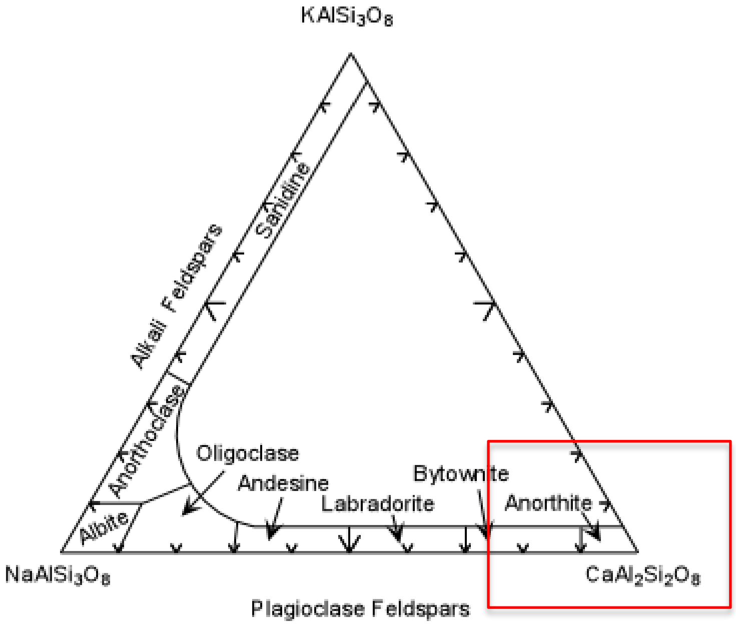


- Important to consider the basic reference frame. i.e. which crystal is basis for calculation?

- One strong OR often introduces another cluster in the data: here γ–α OR and α–α OR

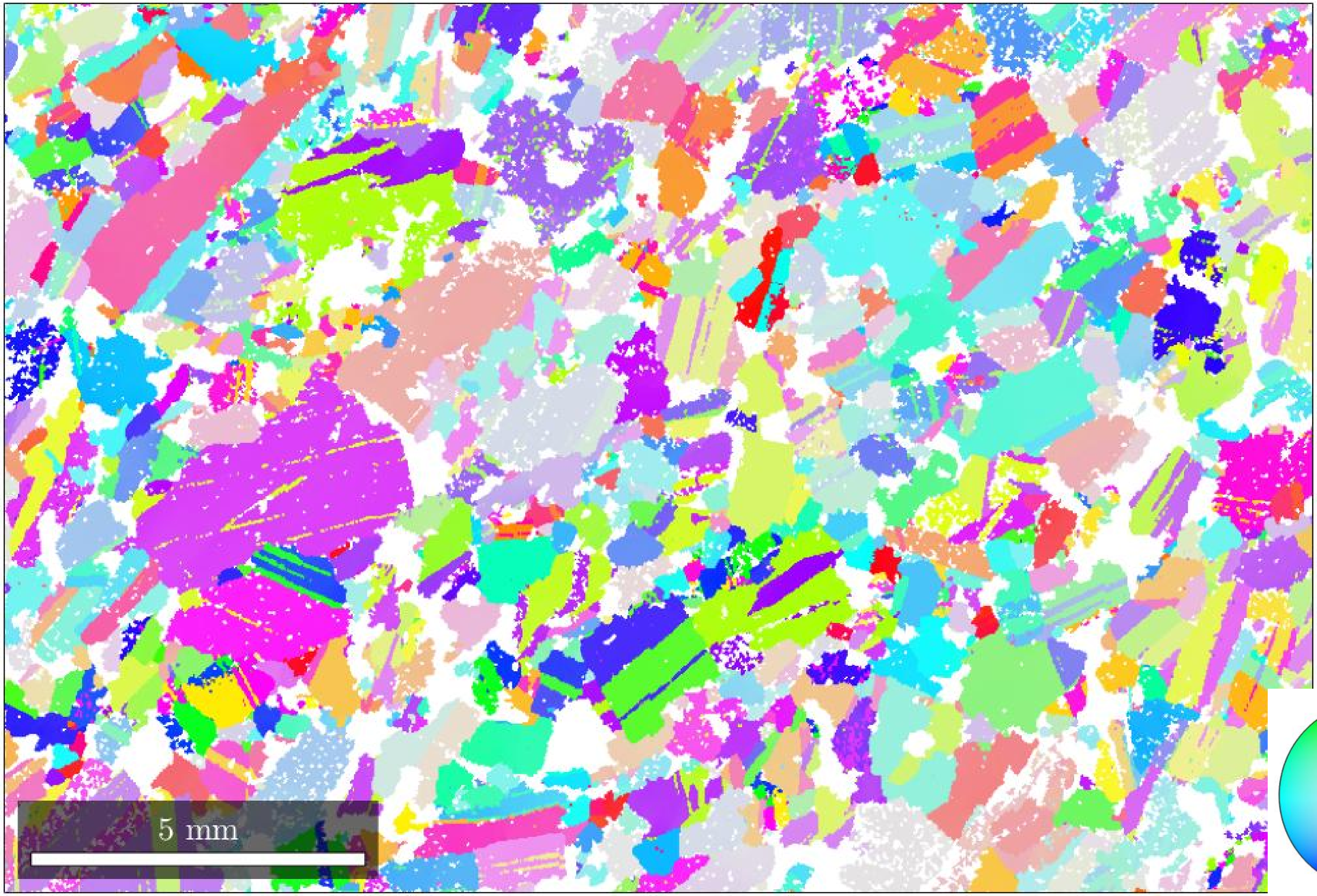
Example 2: Twinning in Anorthite

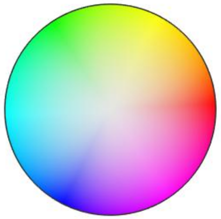
- Anorthite (class of Plagioclase Feldspar)
- High content of Ca and Al, low content of Na and K
- Triclinic crystal structure: -1
- Several known twinning types:
  - Albite 180 degree about (010) normal
  - Manebach 180 degree about (001) normal
  - Carlsbad 180 degree about [001] axis



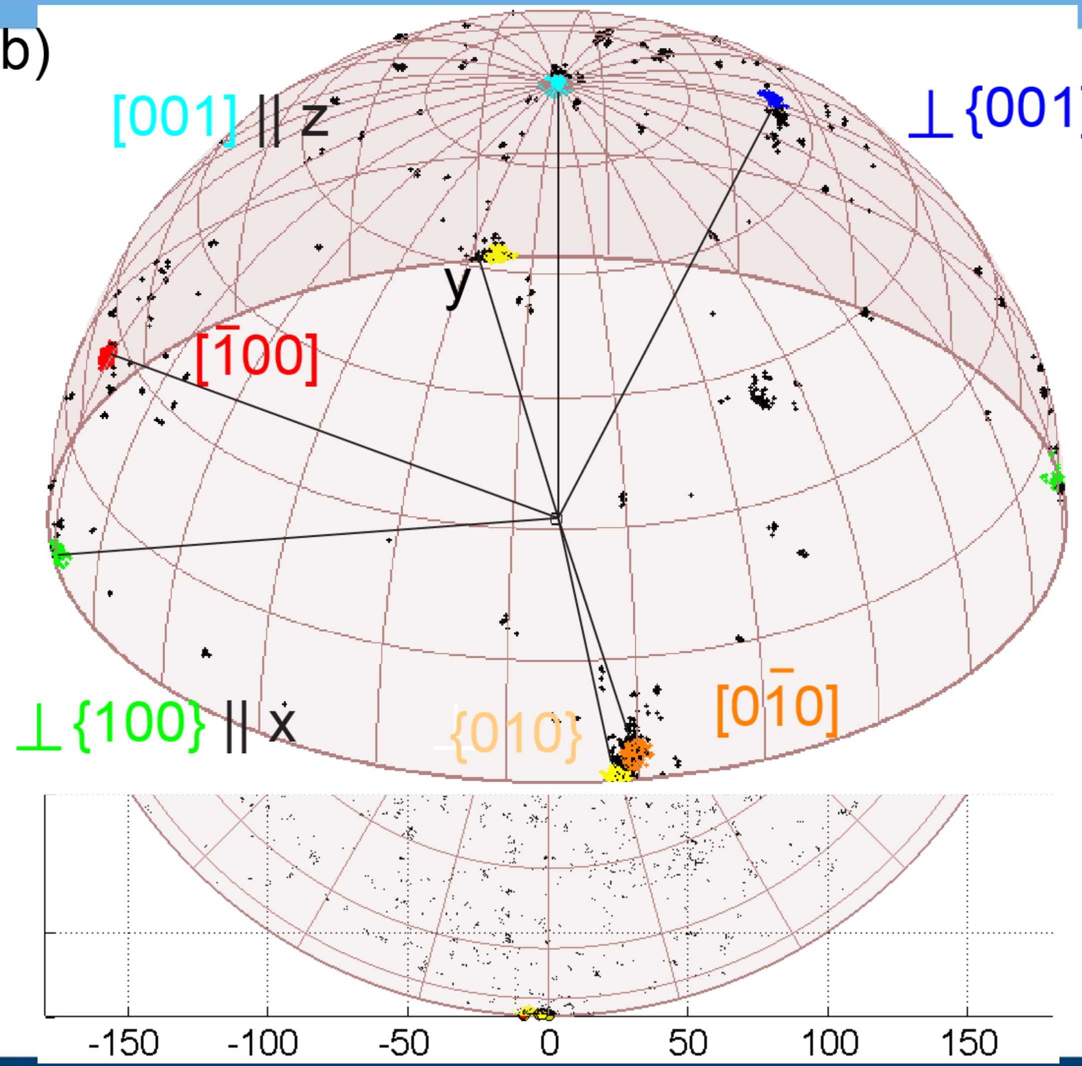
Example 2

(Zoja Vukmanovic, Cambridge)



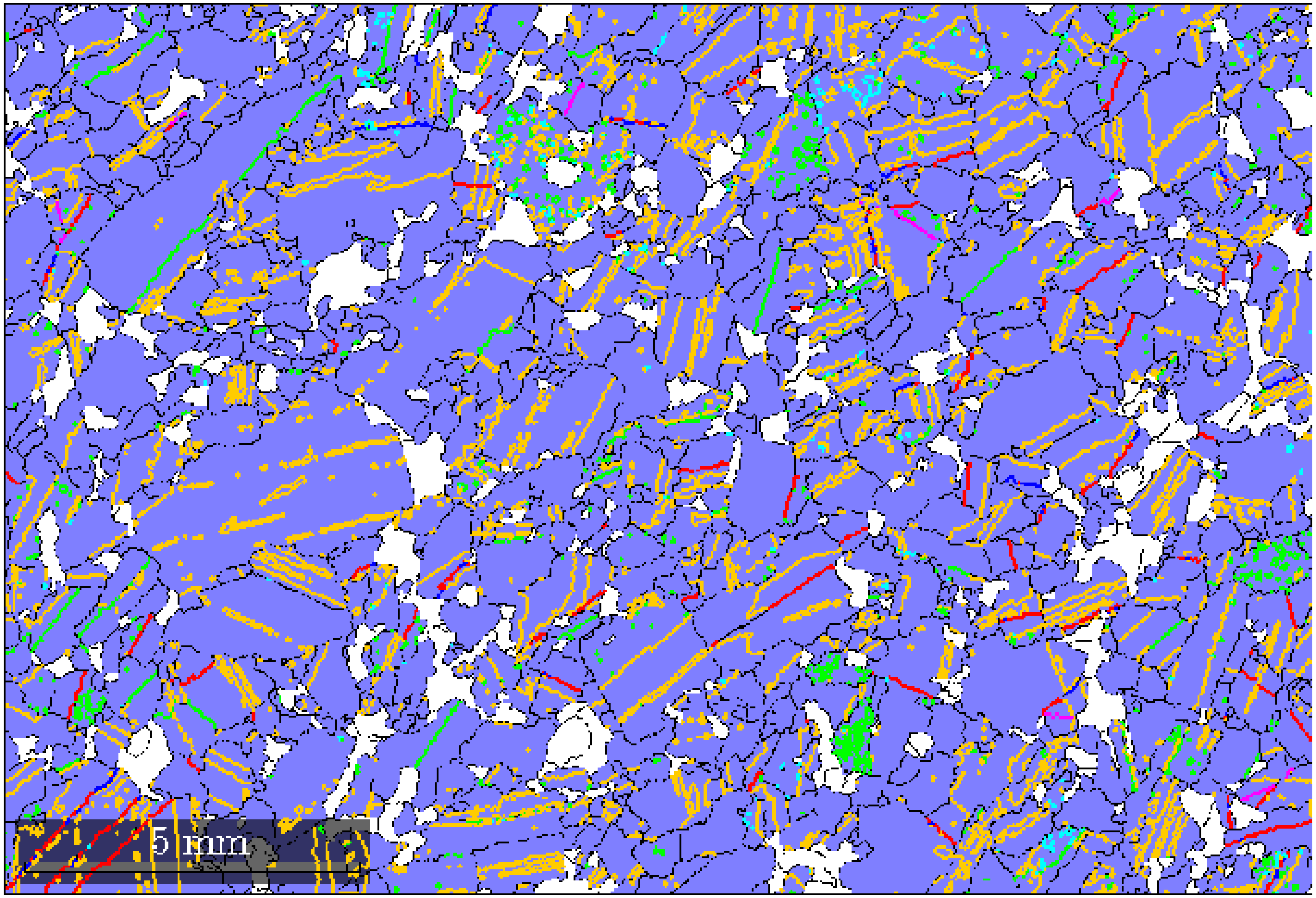


Example 2: Anorthite twins identification, quantify



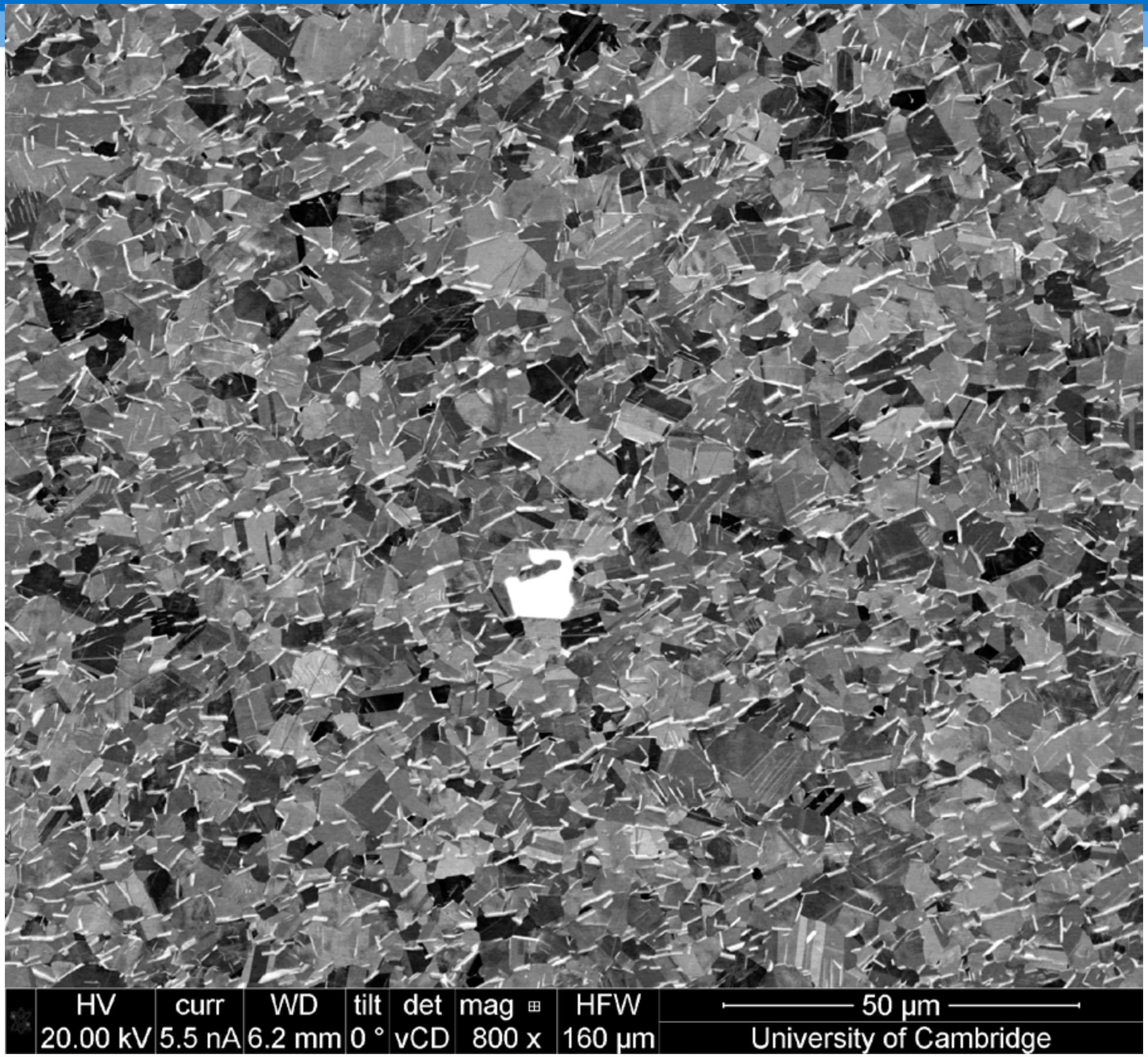
- All common twin types can be identified
  - Red: Ala
  - Green: X-law
  - Yellow: Albite + Pericline
  - Dark Blue: Manebach
  - Black: Carlsbad
- And quantified in terms of relative occurrence

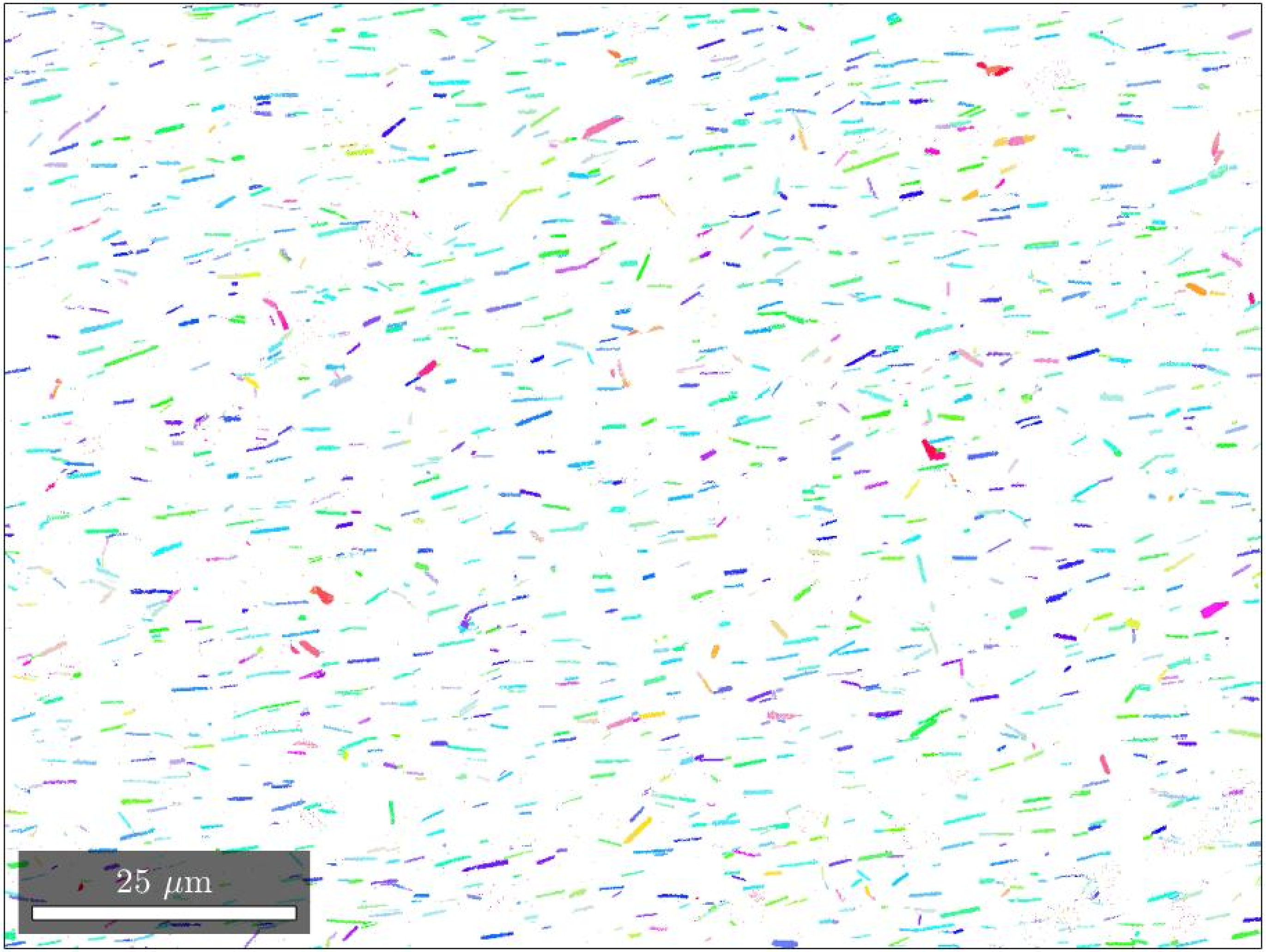
Example 2: Spatial Occurrence

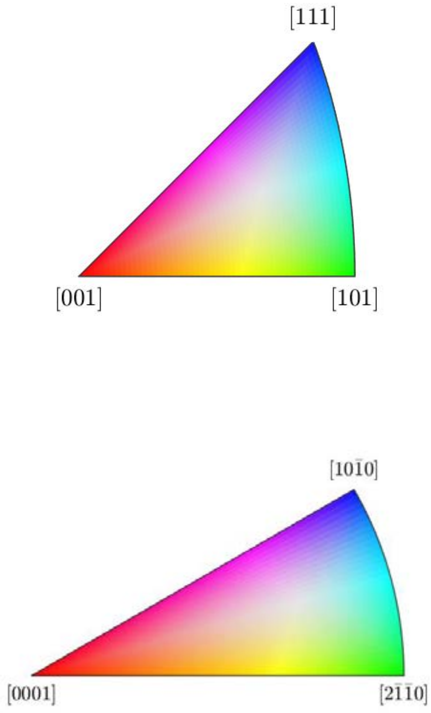


Example 3: Nickel base superalloy 718Plus

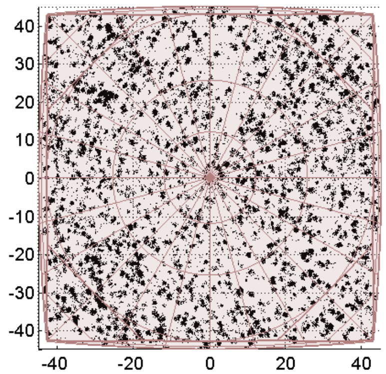
- cubic matrix phase γ (mainly Ni, Cr, Fe, Co)
- precipitate phase η, often at gB (mainly Ni, Nb, Al, Ti)
- Predominant direction → cause: forging operation

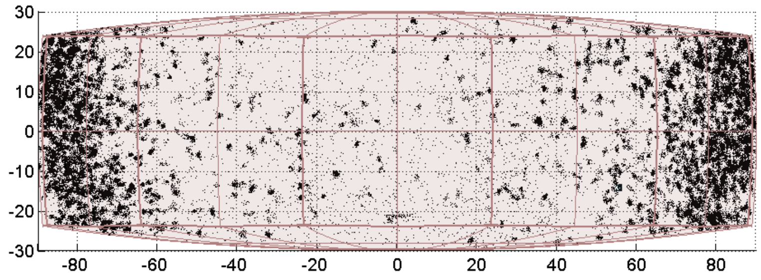


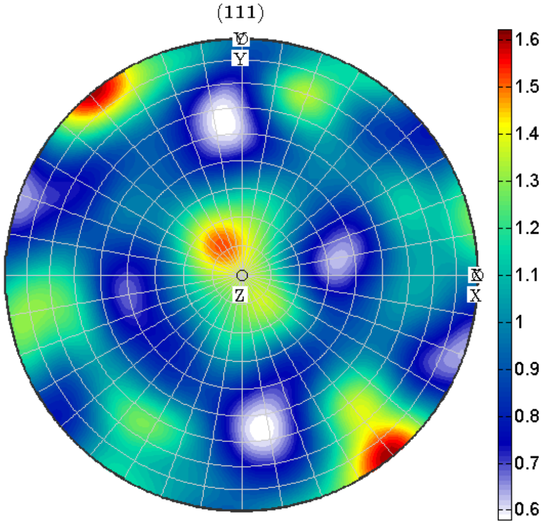

25 μm

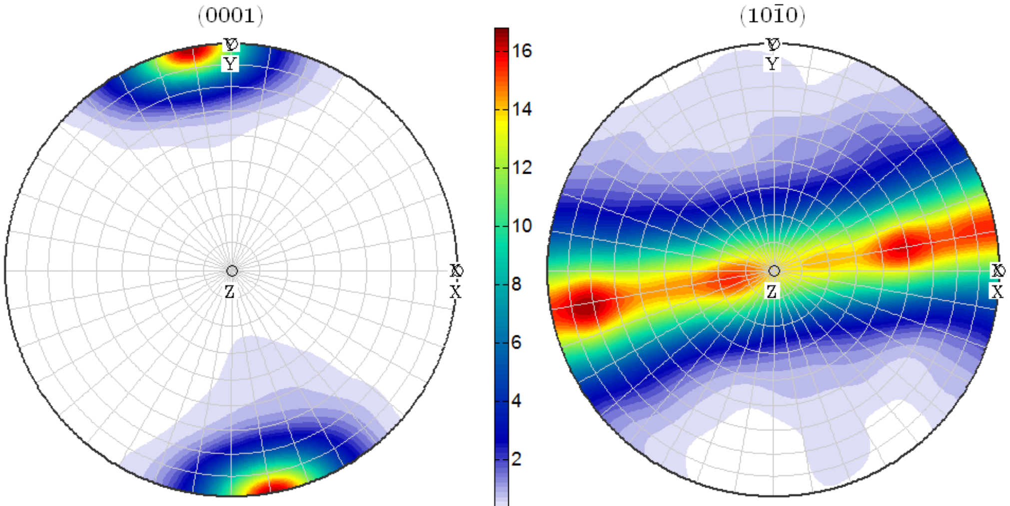

[111]
[001]
[101]
[10$\bar{1}$0]
[0001]
[2$\bar{1}\bar{1}$0]

Texture in Superalloy precipitate

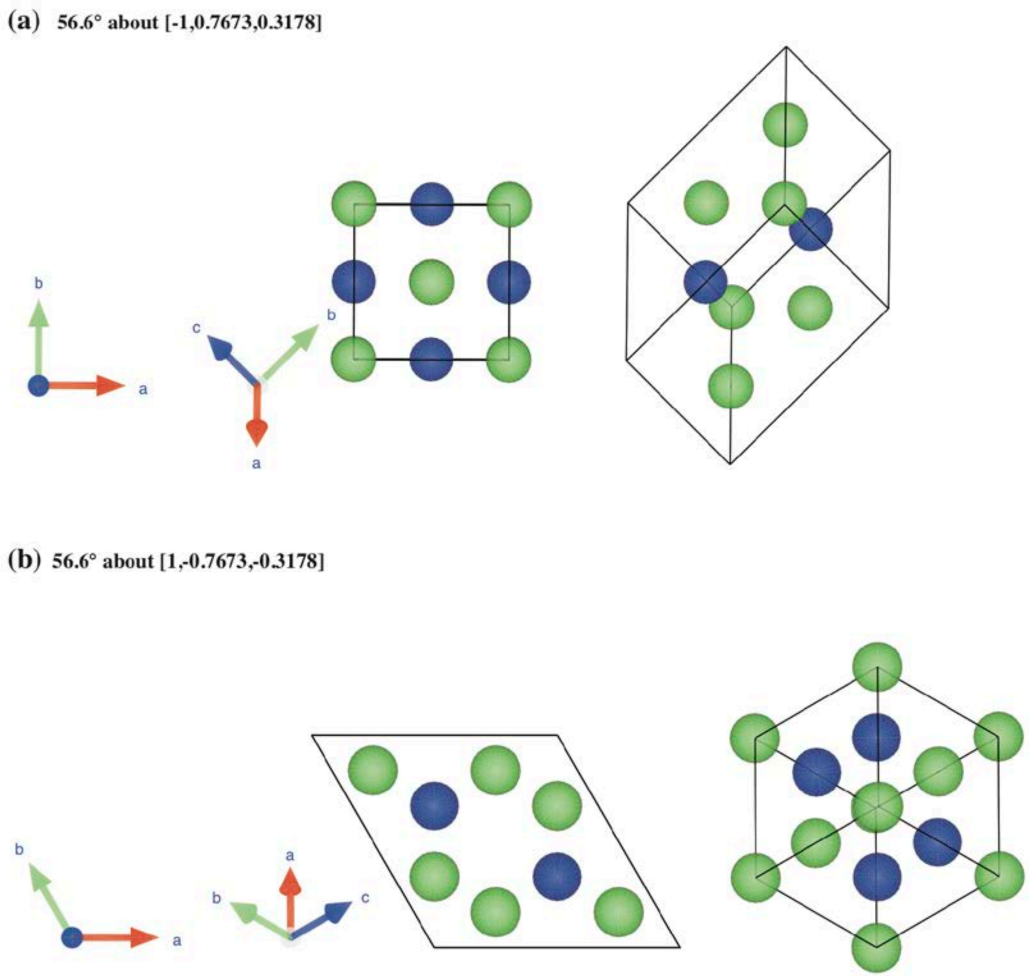




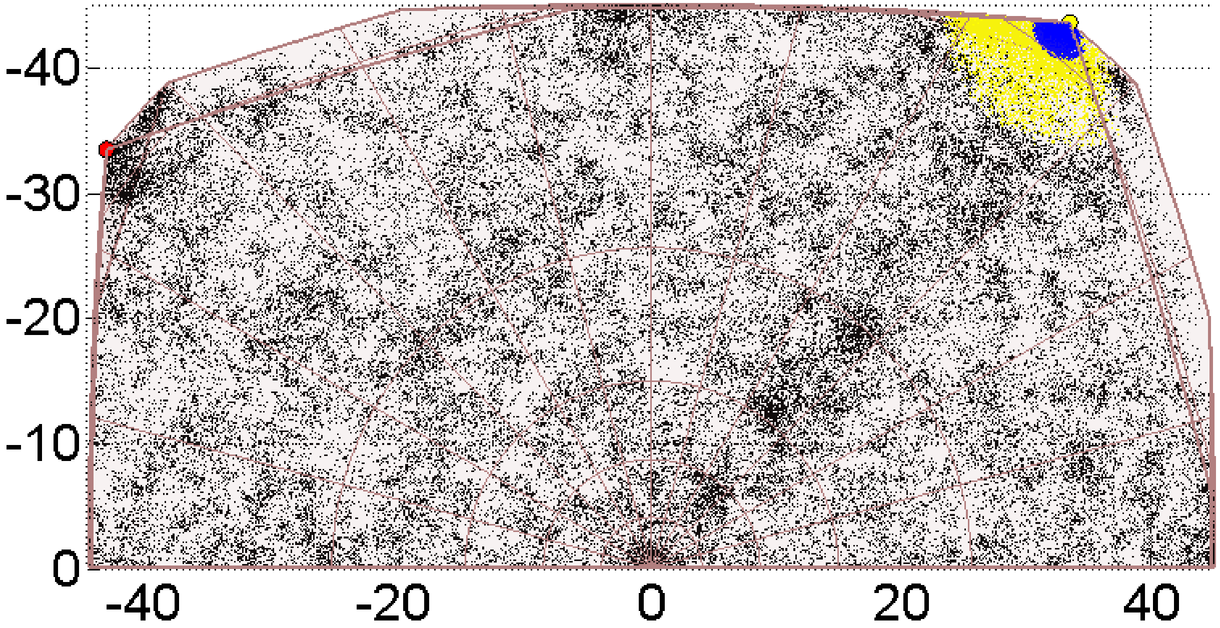


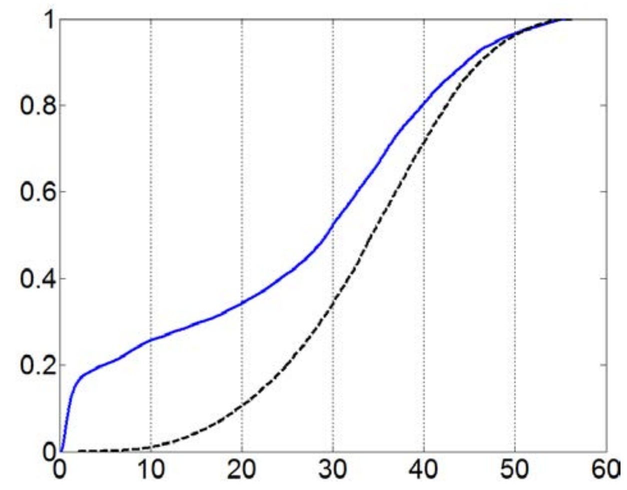


Orientation Relationship - Blackburn



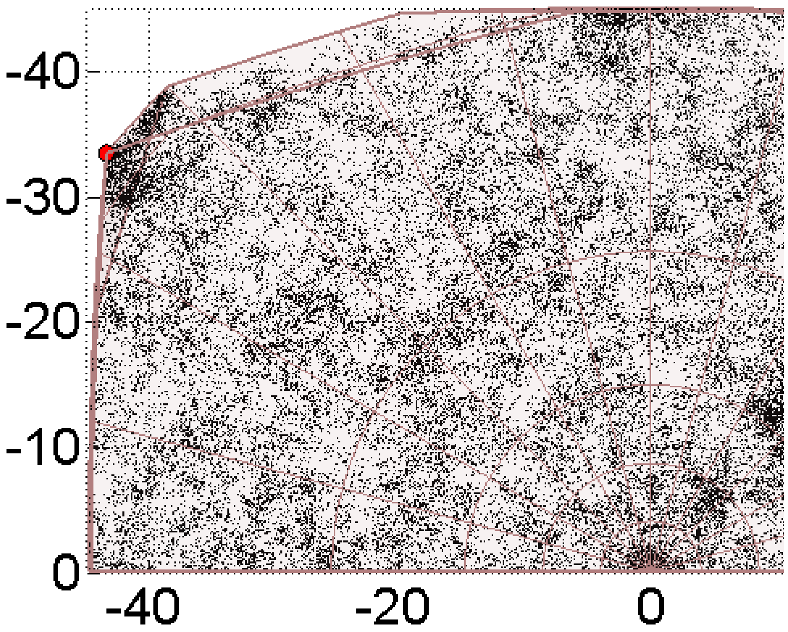
Orientation relationship

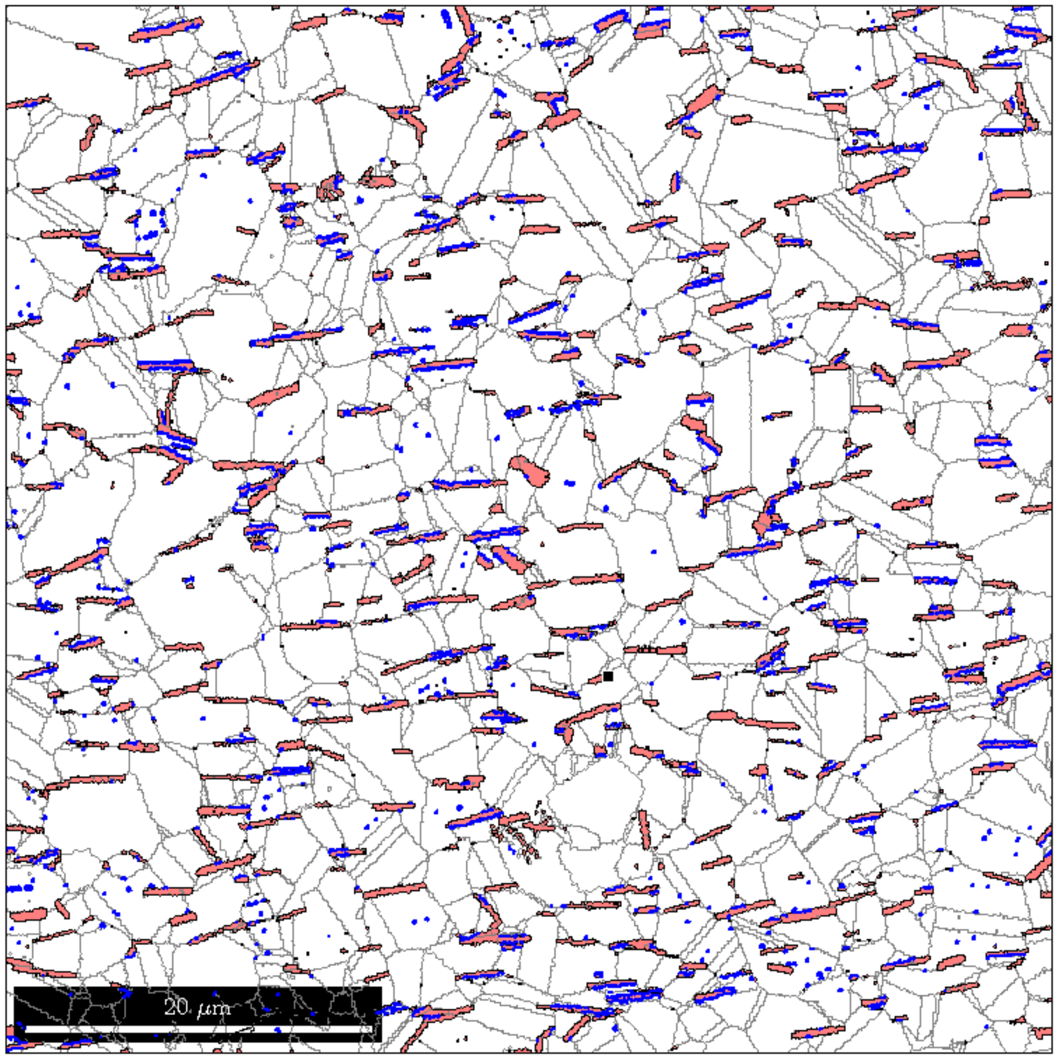




- Two clusters can be identified
- new orientation relationship

Orientation relationship





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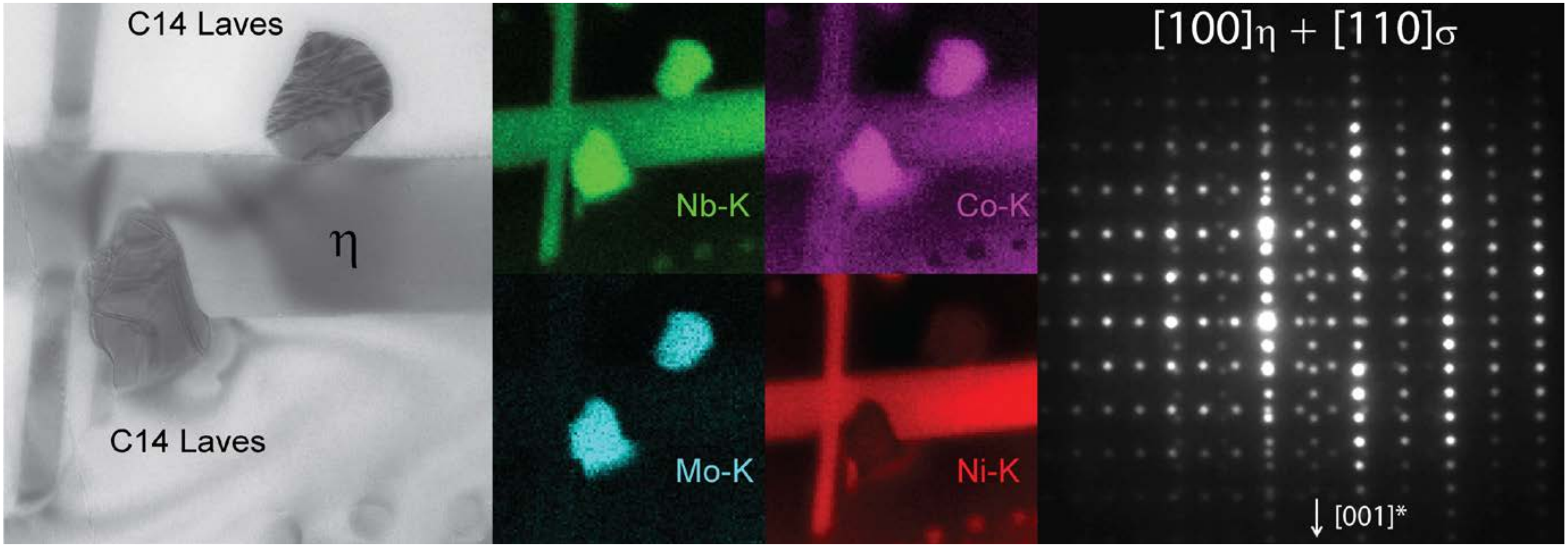
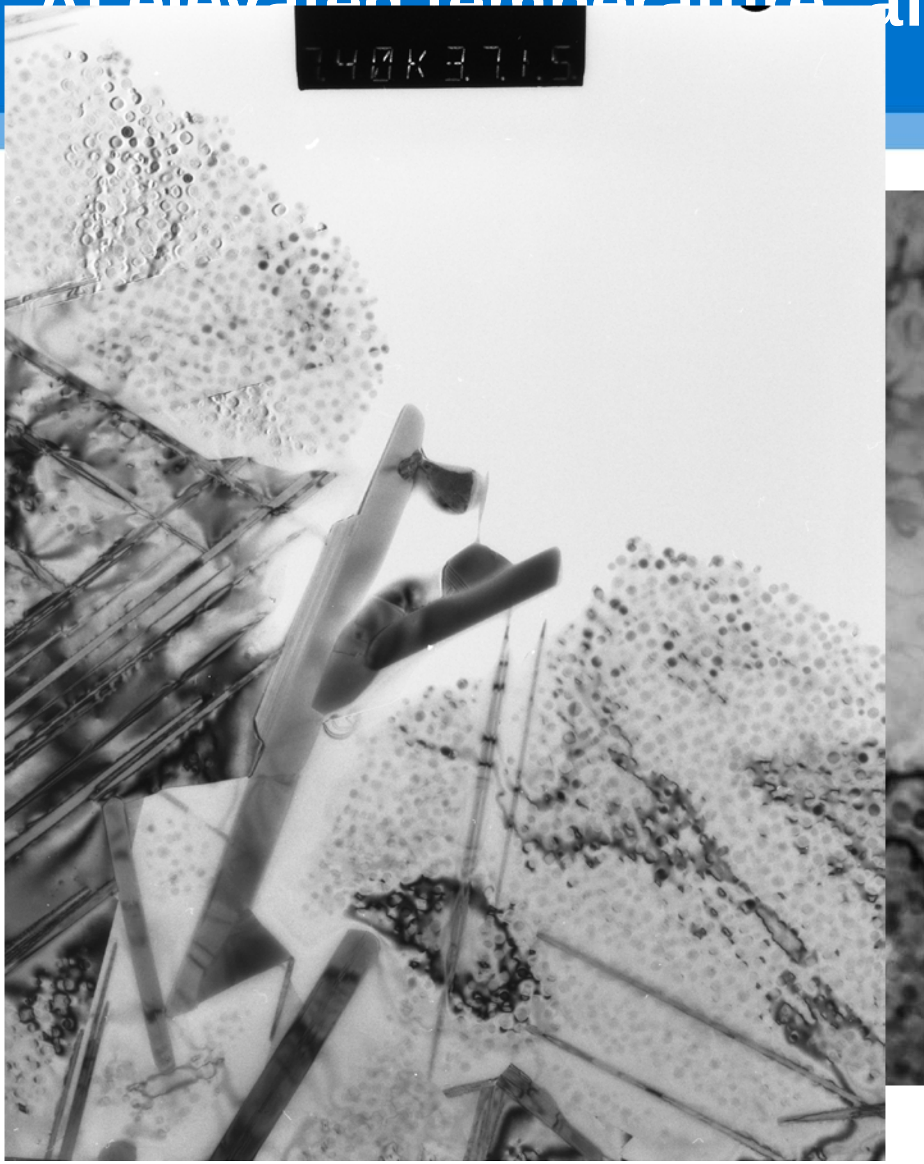
Example 3b

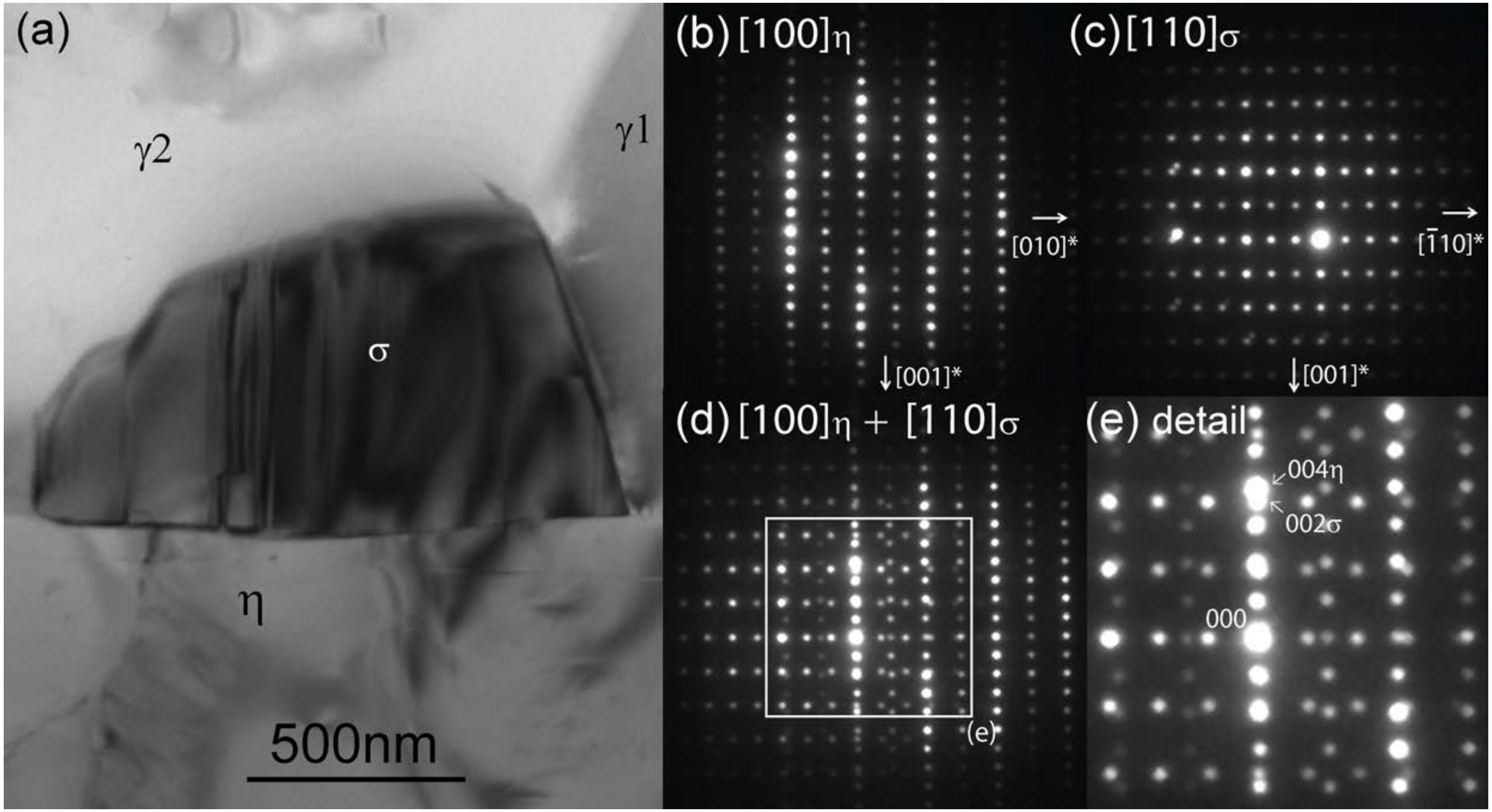


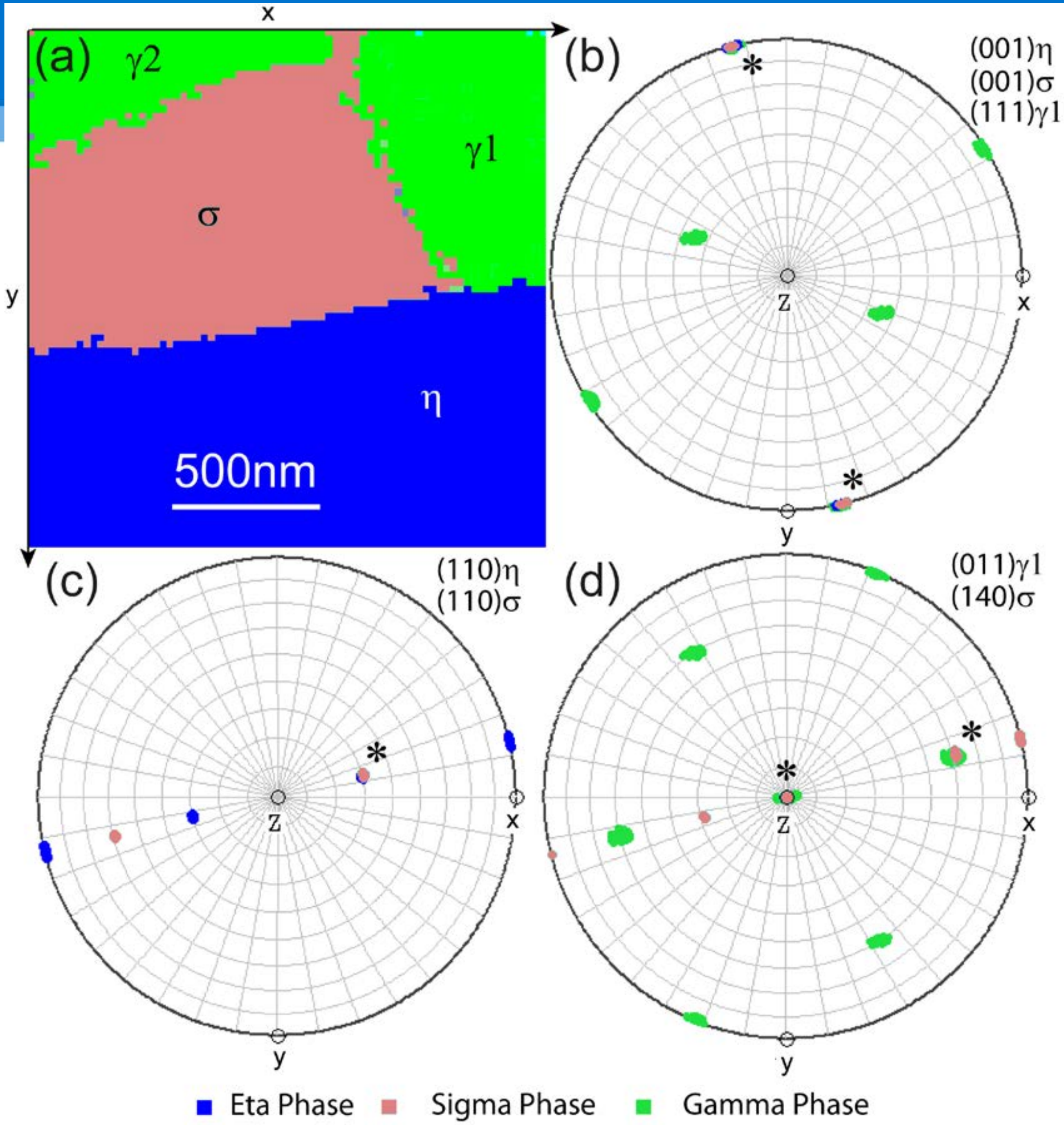
At elevated temperature, after forge + HT



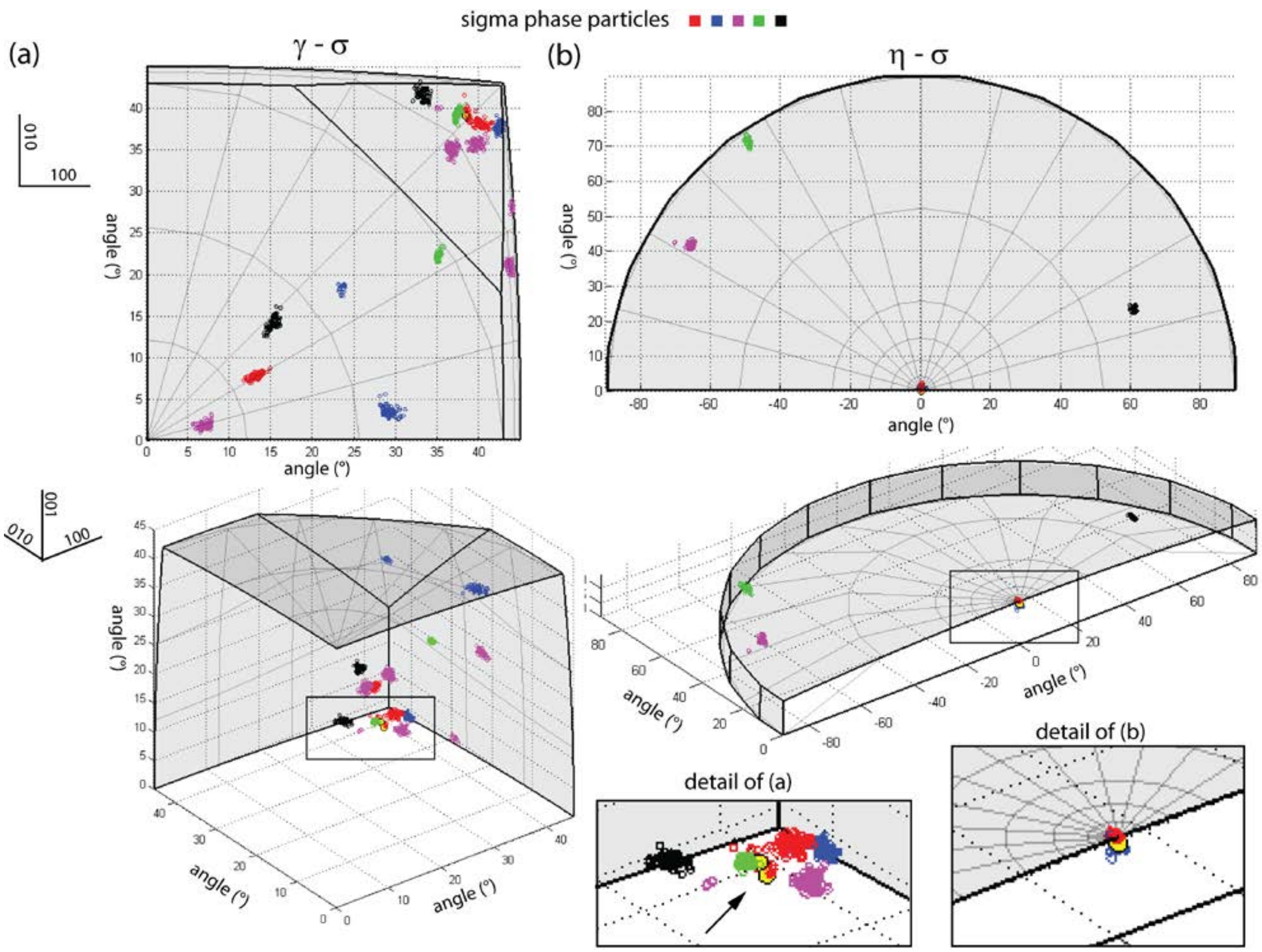
- Unknown phases occurred, rich in matrix elements
- Went to the TEM to study phases using diffraction
- Used SPED, similar to EBSD, but using spot patterns instead of Kikuchi patterns

Sigma Phase – Strong registry with surrounding MS





x
y
(a)
γ2
γ1
σ
η
500nm
(b)
(001)η
(001)σ
(111)γ1
Z
x
y
(c)
(110)η
(110)σ
Z
x
y
(d)
(011)γ1
(140)σ
Z
x
y
Eta Phase
Sigma Phase
Gamma Phase


sigma phase particles
(a)
γ - σ
(b)
η - σ
010
100
001
angle (°)
detail of (a)
detail of (b)

Short Summary

- Orientations and Misorientations are represented in 3 independent variables
    - Ideal to plot in 3D spaces
- Useful to understand your data
    - Mis-indexed data
    - Orientation Relationships (topotaxy)
    - Fibres
    - Size of grains → segmentation angles
- Analyse axis and angle
    - Axis in terms of crystal1, crystal2, specimen reference frame

Summary

- This work demonstrates the usefulness of Neo-Eulerian mappings for insight from orientation and misorientation data through visualisation in 3D spaces.
  - Three examples were discussed showing the successful and robust identification of orientation relationships and texture
  - Axis-angle parametrisation is a good choice for its simple and linear scaling
- In general the features of the (mis-)orientation data are indicated by clusters in the (mis-)orientation spaces
  - Perhaps, the development of specialised clustering algorithms would be valuable.
- A key feature of the analysis workflows presented is also that correlations are drawn between the orientation space information and the real space spatial information.
- Overall, it is shown that these techniques provide an elegant and insightful representation of the data that can make seemingly overwhelming quantities of orientation data manageable.

Acknowledgement

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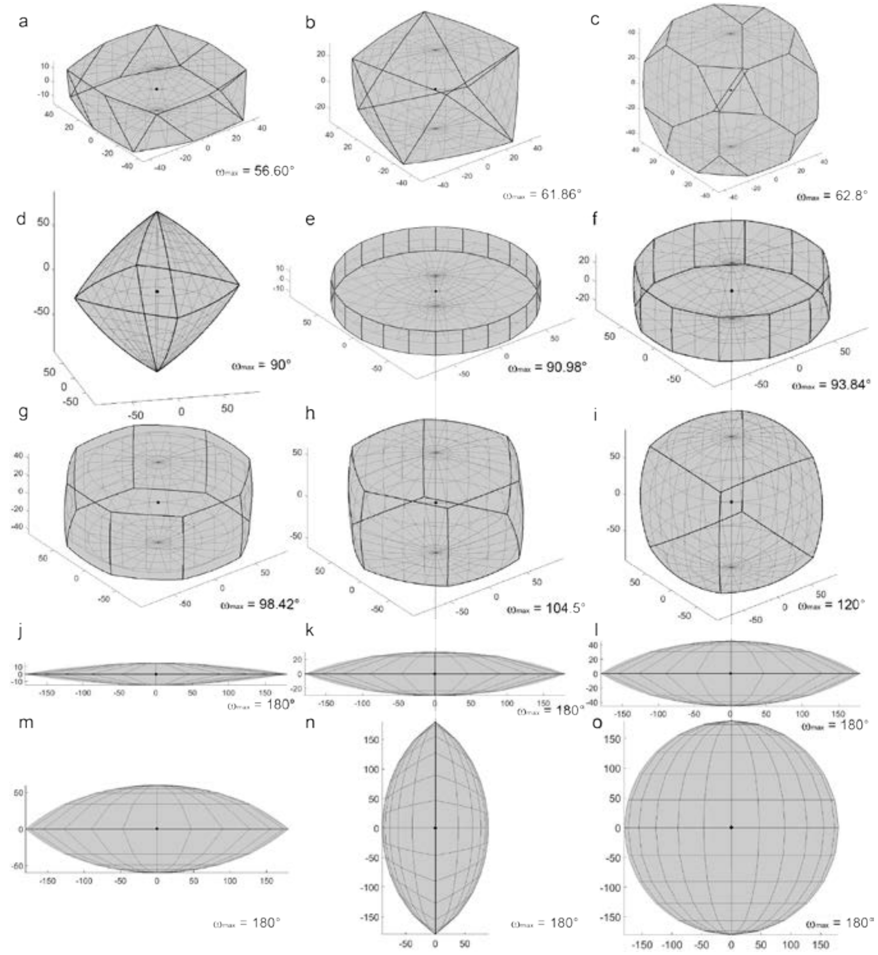
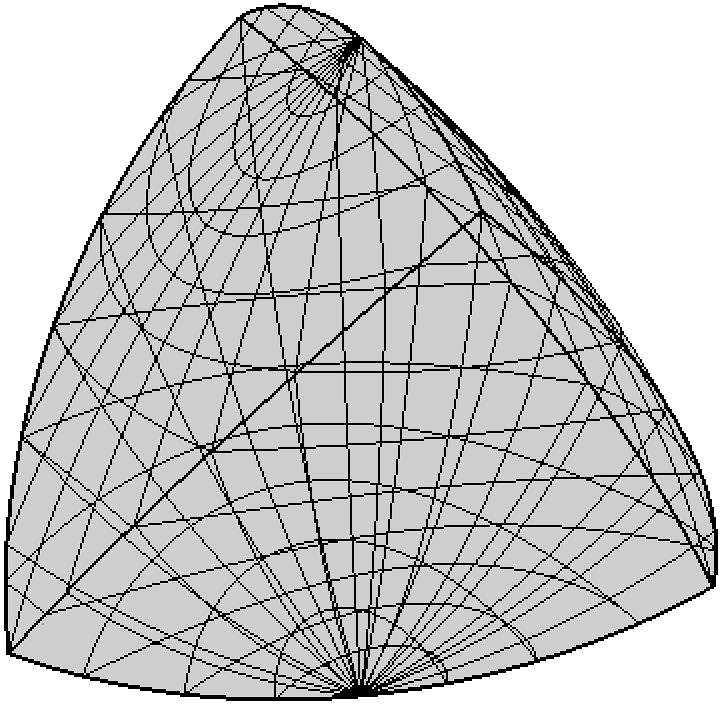
- Permission to publish this article has been given by Rolls-Royce plc.
- Requests for access to the underlying research data should be directed to the corresponding author and will be considered against commercial interests and data protection.

Backup: 15 unique spaces

- 15 unique spaces
  - Characterised by the max misorientation angle
  - Depend on setup of reference frames
- Sections exist as well



Different Choice of Reference Frames



Twinning in Titanium