Representing Orientations and Misorientations

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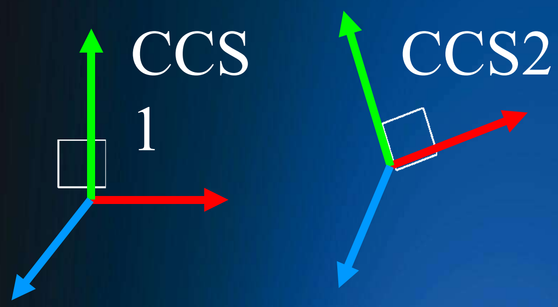
Representing Orientations

- Specification of the relationship between two different coordinate systems
  - sample coordinate system (SCS)
  - crystal coordinate system (CCS)

Representing Misorientations

- Specification of the relationship between two different coordinate systems
  - crystal coordinate system for crystal 1 (CCS1)
  - crystal coordinate system for crystal 2 (CCS2)



So most representations are applicable to both orientations and misorientations, although some are more convenient for one or the other

Representing (Mis)Orientations

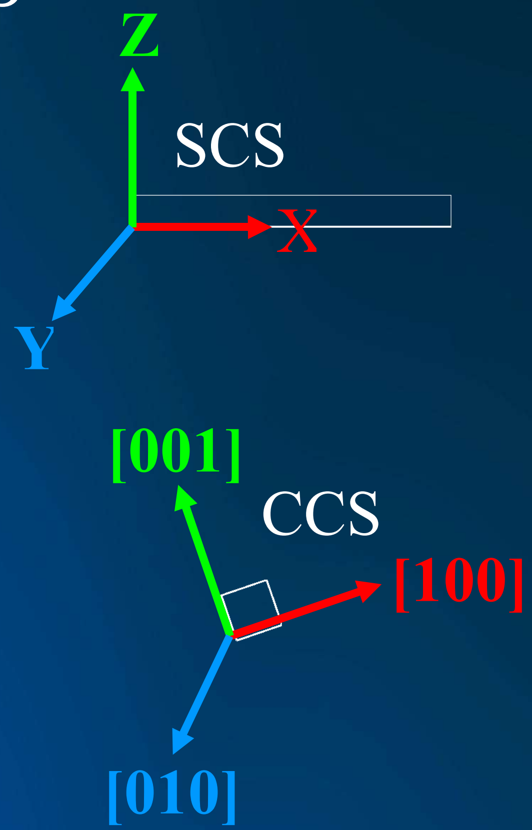
- The relationship between the two coordinate systems may be specified by:
  - Rotation matrix
  - Miller indices → Pole Figures
  - Euler angles → Euler Space (ODFs)
  - Angle/axis of rotation → Rodrigues Space
  - Rodrigues vector → Rodrigues Space
  - Quaternion

This presentation covers the methods in yellow, which are the main methods used in the Channel software

Rotation Matrix (1)

- The rotation of the sample axes onto the crystal axes, i.e. CCS = g . SCS

$$g = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} \cos\alpha_1 & \cos\beta_1 & \cos\gamma_1 \\ \cos\alpha_2 & \cos\beta_2 & \cos\gamma_2 \\ \cos\alpha_3 & \cos\beta_3 & \cos\gamma_3 \end{pmatrix}$$



$\alpha_1, \beta_1, \gamma_1$ are angles between [100] and X, Y, Z

$\alpha_2, \beta_2, \gamma_2$ are angles between [010] and X, Y, Z

$\alpha_3, \beta_3, \gamma_3$ are angles between [001] and X, Y, Z

Rotation Matrix (2)

- **Fundamental:** the other representations of orientation / misorientation can be derived from it
- **Rarely seen:** the other representations are usually better for visualising and / or analysing orientations / misorientations

Miller Indices (Ideal Orientation)

- (hkl)[uvw] where (hkl)||rolling plane, [uvw]||rolling direction *
- {hkl}<uvw> for a Miller indice family
- For a **cubic crystal structure**, (hkl)[uvw] is equivalent to [hkl]||Z and [uvw]||X

* Convention for rolled samples. For other samples, replace "rolling plane" with "plane⊥Z" and rolling direction with "X".

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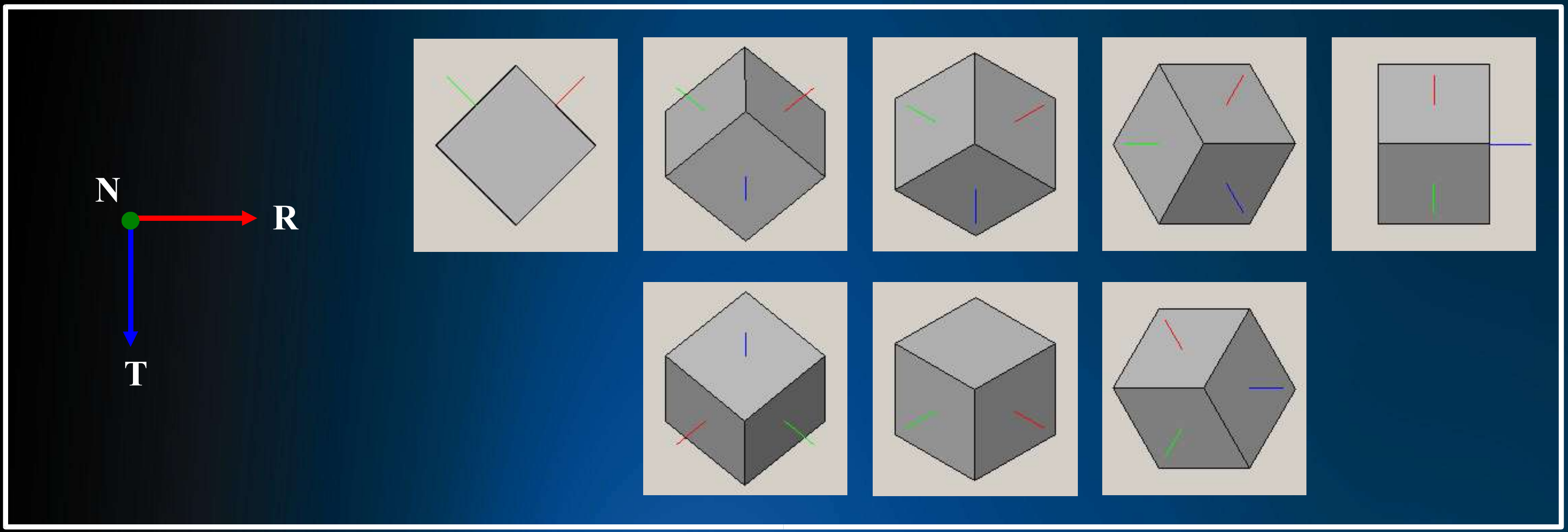
Examples – Miller Indices

{001}<110> {112}<110> {111}<110> {111}<112> {110}<001>



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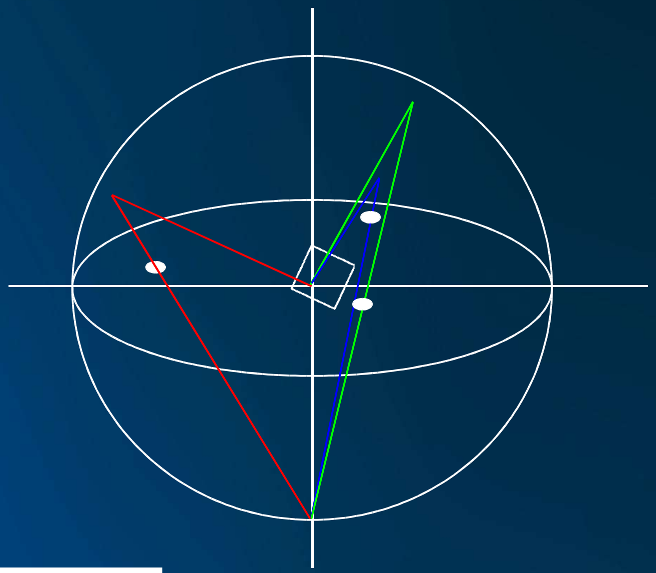
Pole & Inverse Pole Figures

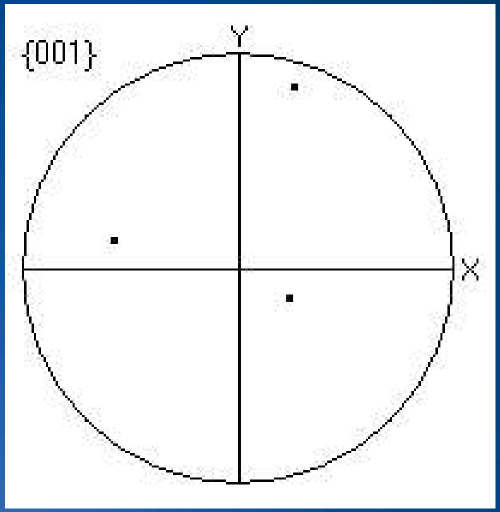
- Pole figures are a description of the crystal orientation(s) with respect to the sample coordinate system
- Inverse pole figures are a description of the sample orientation with respect to the crystal coordinate system(s)
- PF / IPF description of orientation may be ambiguous (e.g. <0001> PF, single IPF)

Pole Figures

- Projection of poles (normals to crystallographic planes) onto a sphere, then onto a plane
- In metallurgy, use upper hemisphere and stereographic projection

Upper hemisphere, stereographic projection of {001} poles

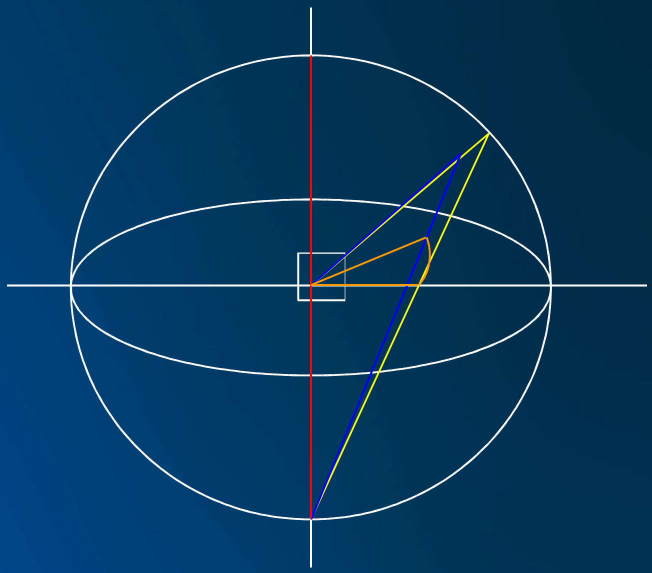


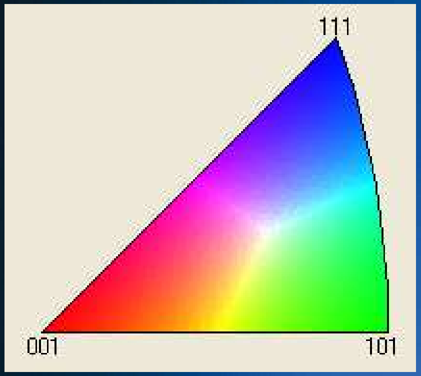


Resulting {001} pole figure

Inverse Pole Figures (1)

- Projection of a sample axis onto a sphere, then onto a plane
- In metallurgy, use upper hemisphere and stereographic projection





With cubic crystal symmetry, all possible orientations of a single direction can be displayed in a "triangle" (left) defined by projections of the <001>, <101> and <111> directions of an {001}<100> cube (above)

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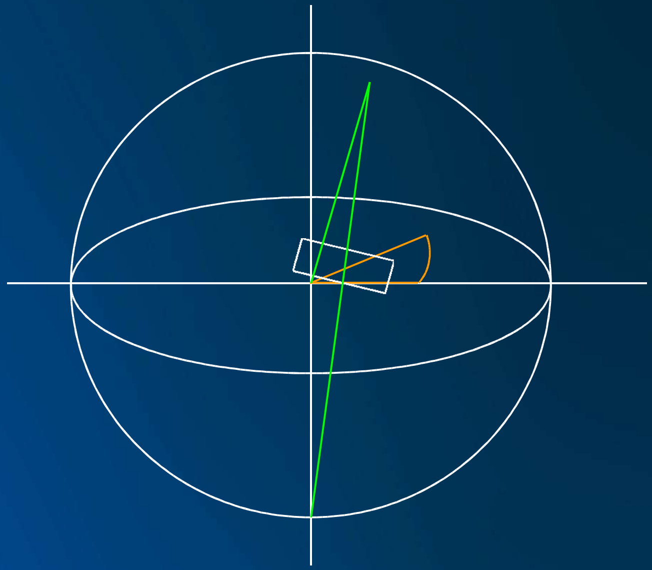
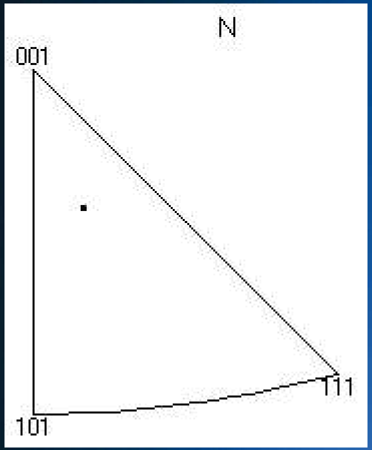
Inverse Pole Figures (2)

- Need one IPF for each direction of importance
- Individual orientations still ambiguous unless labelled

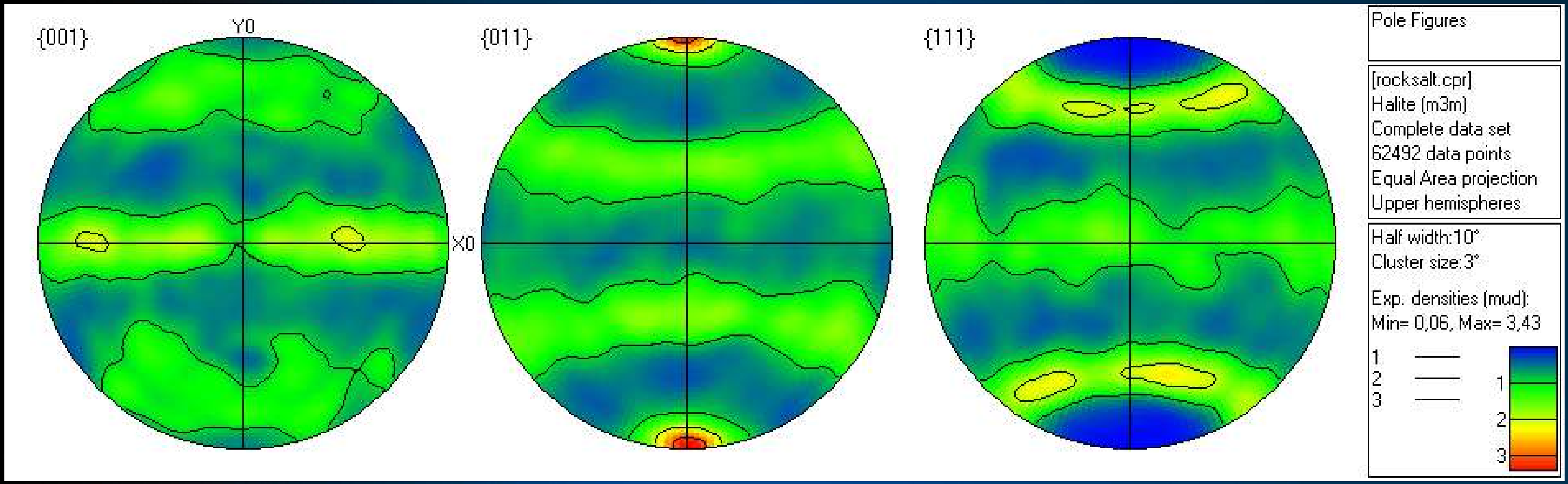


Upper hemisphere, stereographic projection of sample normal direction



Resulting ND inverse pole figure

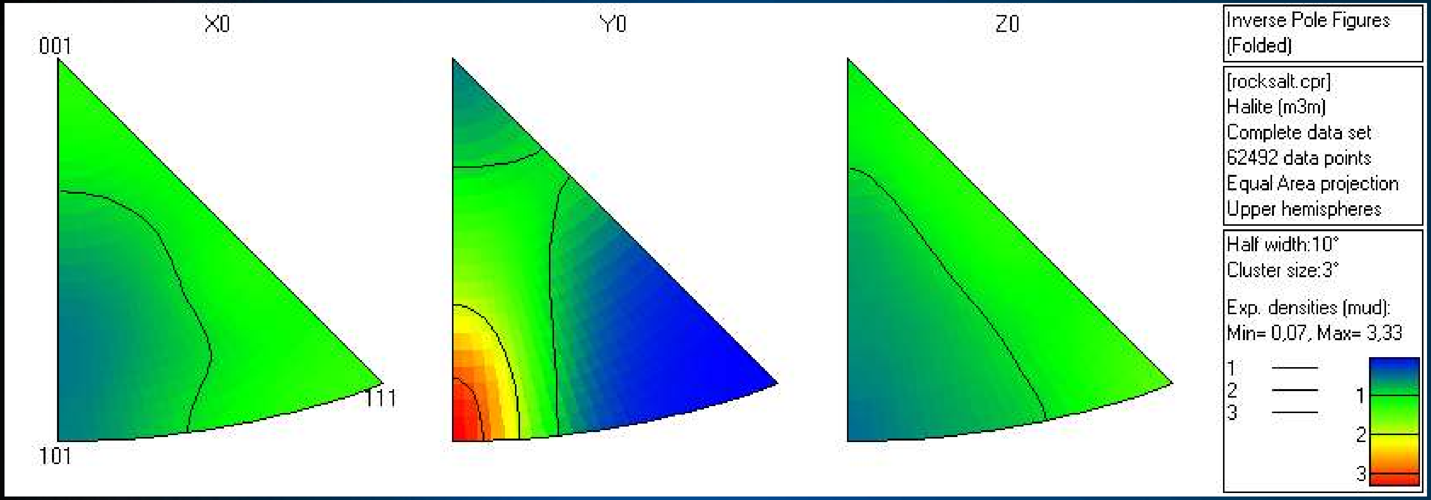
Example – Pole Figures



{100}, {110} and {111} pole figures for a sample of experimentally-deformed rocksalt

The sample has a fibre texture with <011>||Y0

Example – Inverse Pole Figures



Inverse pole figures for the same sample of experimentally deformed rocksalt

The dominant fibre texture is clear in the Y0 figure

Euler Angles

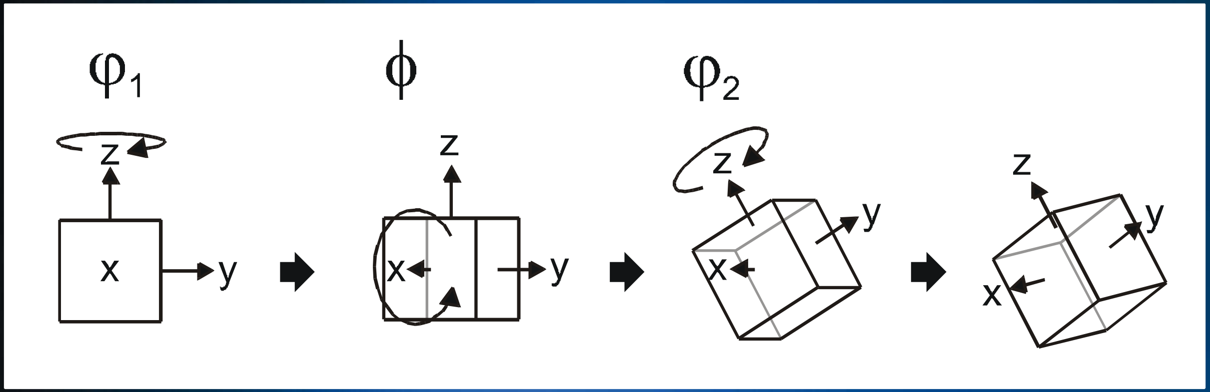
- Three angles specifying the rotation of the sample axes onto the crystal axes
- Bunge convention is most common

∀ ϕ_1 about Z

∀ Φ about X (in its new position)

∀ ϕ_2 about Z (in its new position)

- Must be performed in the given sequence



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Euler Space & ODFs (1)

- 3-D orientation space with mutually perpendicular axes for ϕ_1, Φ, ϕ_2
- Discrete orientations are represented by points in Euler space
- Textures are represented by contours in Euler space formed by mathematical smoothing of the discrete orientation data to give Orientation Distribution Functions (ODFs)

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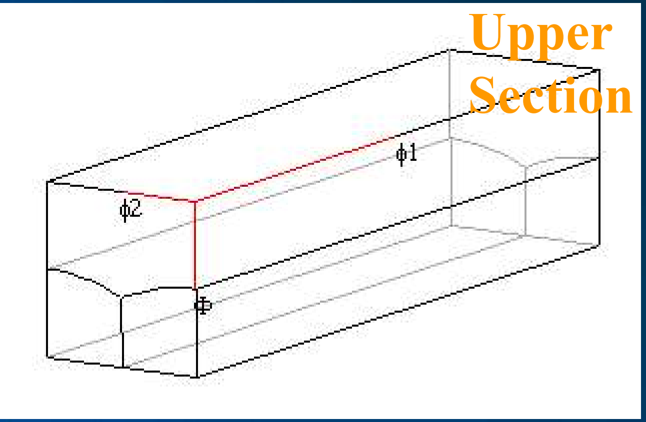
Euler Space & ODFs (2)

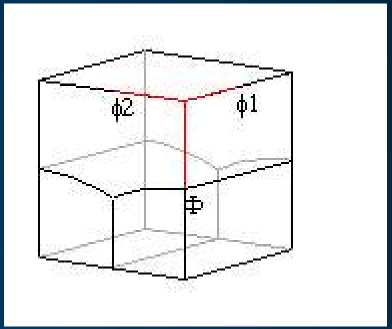
- For the most general case, **triclinic crystal symmetry** & **no sample symmetry**, Euler angle limits are
  $0° \le \varphi_1 \le 360°$, $0° \le \Phi \le 180°$, $0° \le \varphi_2 \le 360°$
- For **cubic crystal symmetry**, each orientation can be represented by an equivalent in the space
  $0° \le \varphi_1 \le 360°$
  $0° \le \Phi \le \mathrm{acos}\,[\cos\varphi_2/\sqrt{(1+(\cos\varphi_2)^2)}]$ for $0° \le \varphi_2 \le 45°$
  $0° \le \Phi \le \mathrm{acos}\,[\cos(90-\varphi_2)/\sqrt{(1+(\cos(90-\varphi_2))^2)}]$ for $45° \le \varphi_2 \le 90°$
  $0° \le \varphi_2 \le 90°$
  but it is more common to use
  $0° \le \varphi_1 \le 360°$
  $0° \le \Phi \le 90°$
  $0° \le \varphi_2 \le 90°$
  which contains 3 crystallographic equivalents for each orientation

Entire Space



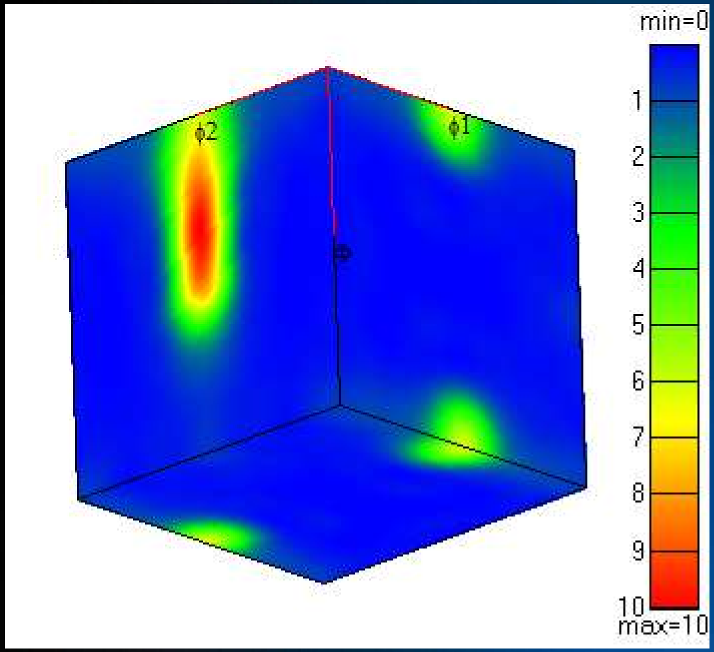
Euler Space & ODFs (3)

- For **cubic crystal symmetry** and **orthorhombic sample symmetry** the limit on ϕ_1 can be reduced to: $0° \leq \varphi_1 \leq 90°$



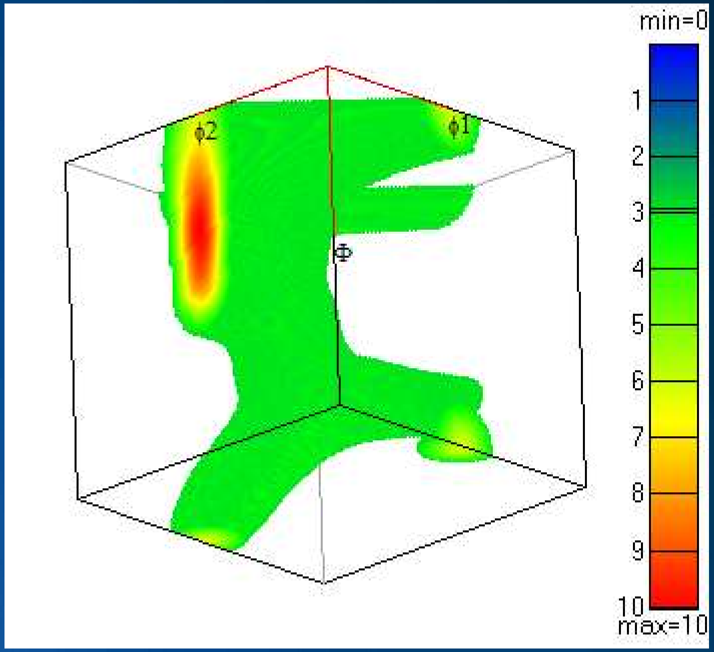
- Advantages of Euler Space
  - Accurate representation of orientation data in 3D (but usually reduced to 2D sections for publication)
- Disadvantages of Euler Space
  - Individual sections bounded by curved surfaces
  - Std prism for cubics displays 3 points per orientation
  - Fibres are usually curved
  - Not homochoric – geometric distortion

Example – ODF in 3D



ODF of a cold-rolled steel

Main texture fibres in 3D



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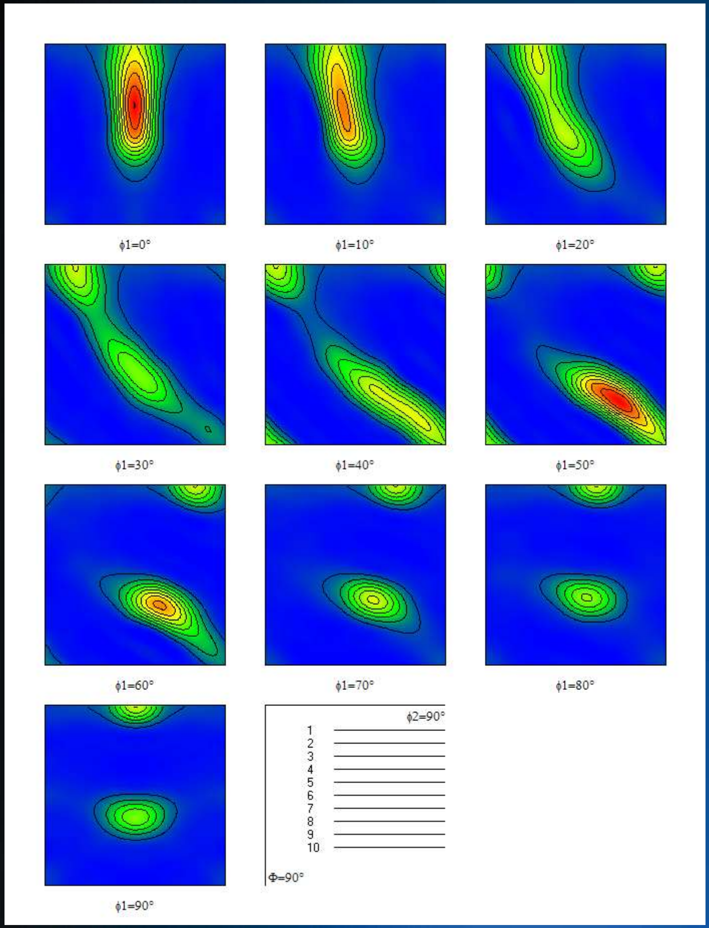
Example – ODF Sections

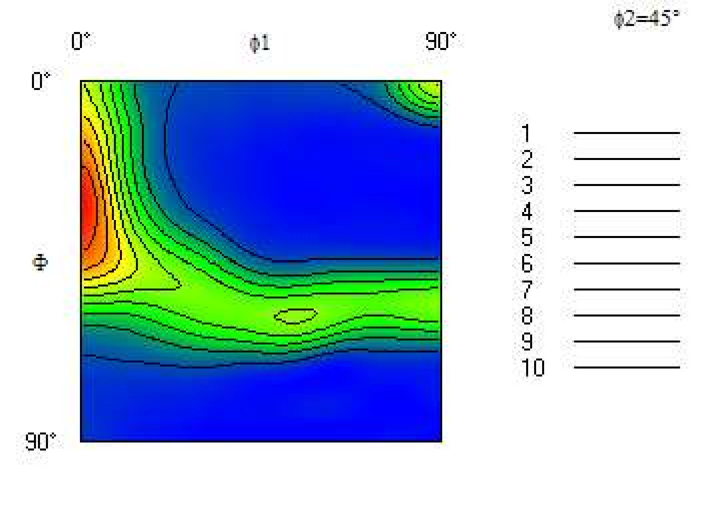


ϕ1 = 0, 10, 20, ..., 90° sections

ϕ2 = 45° section

RD-fibre (<110>||RD) along ϕ1 = 0°

ND-fibre (<111>||ND) along Φ = 55°



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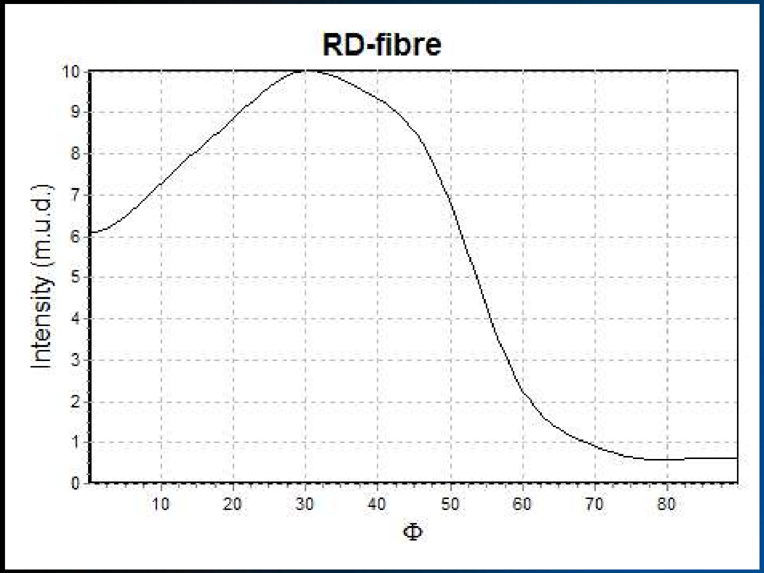
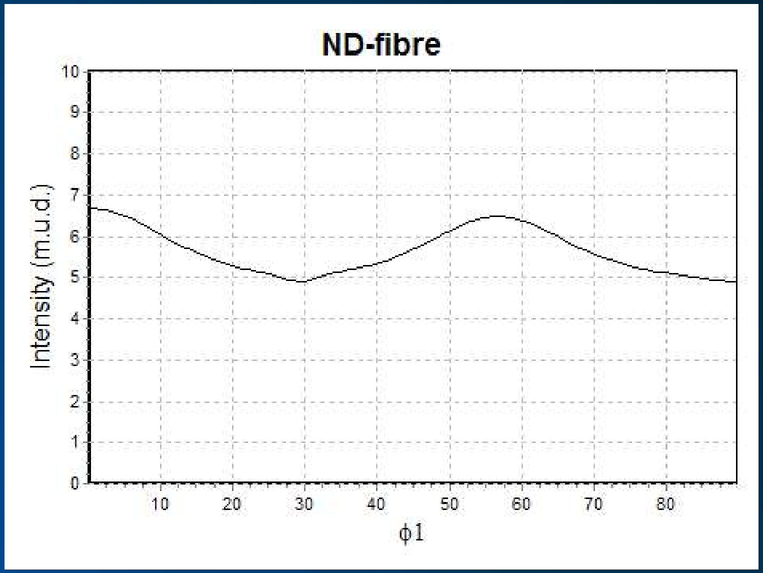
Example – ODF Profiles



Intensity along RD-fibre (<110||RD>)

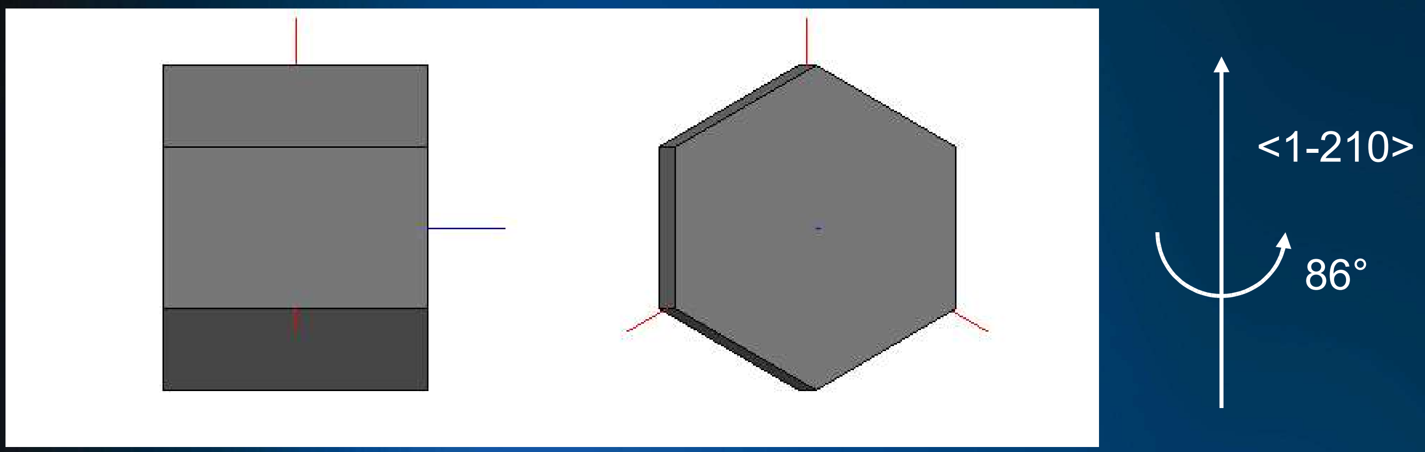


Intensity along ND-fibre (<111||ND>)

Angle/Axis of Rotation

∀ ω°<uvw>

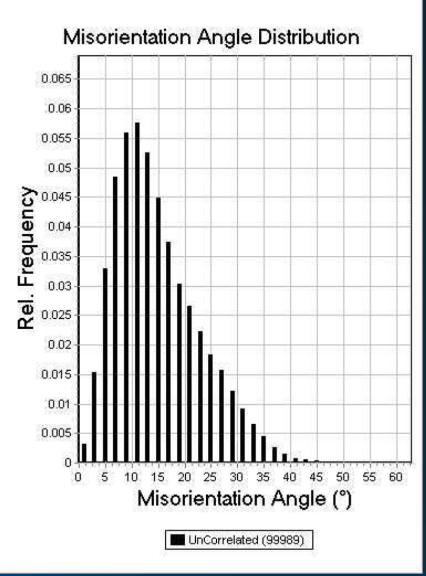
- More commonly used for misorientations
- Can be derived from the orientation matrix

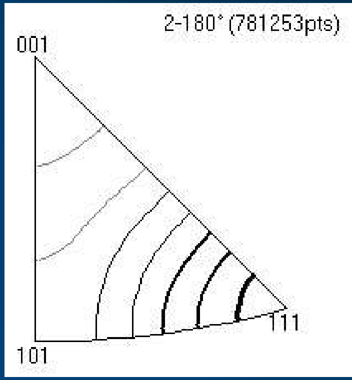


86° <1-210> misorientation caused by a common twinning mode in magnesium

Example – Angle/Axis

- Misorientation Angle Distributions
  - Graph of frequency vs angle, ω°
  - Minimum angle representation
- Misorientation Axis Distributions
  - Axes for a certain angular range plotted on PFs or IPFs
- Depending on purpose, use
  - Spatially-correlated misorientations
  - Spatially-uncorrelated misorientations





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