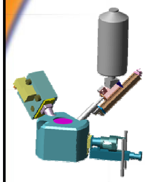
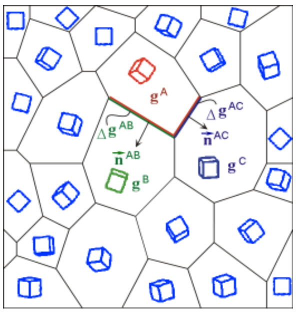
Crystallographic orientation



Orientations and misorientations



Orientation (g):
The orientation of the crystal lattice with respect to some reference frame; usual a frame defined by the processing or sample geometry.

Misorientation (Δg):
The orientation of one crystal lattice with respect to another. Some times termed the orientation difference or disorientation.

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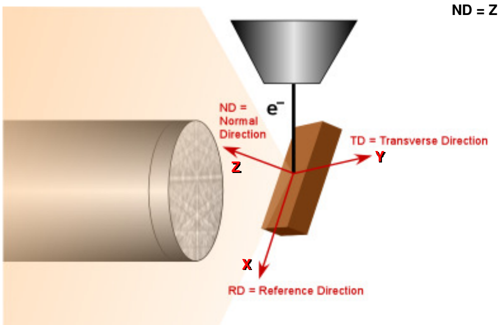
Reference frame

RD = X = [100]
TD = Y = [010]
ND = Z = [001]



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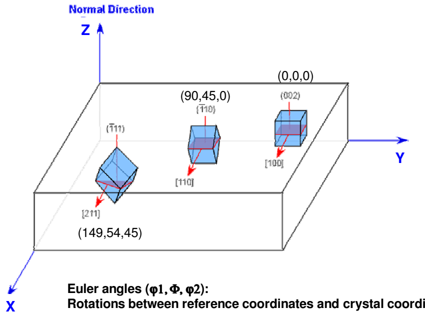
Orientations



Euler angles
($\varphi_1, \Phi, \varphi_2$)

{hkl}<uvw>

Euler angles ($\varphi1, \Phi, \varphi2$):
Rotations between reference coordinates and crystal coordinates

{hkl}<uvw>
Orientation defined by plane {hkl} // specimen surface and crystal direction <uvw> // RD (X)

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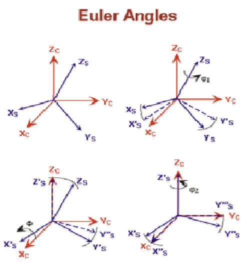
Euler angles



OIM follows the formalism of Bunge (Texture Analysis in Materials Science, Butterworths, 1982).

The three Euler angles ($\varphi_1, \Phi, \varphi_2$) describe the three rotations that will bring the sample reference frame (S) into coincidence with the crystal reference frame (C).

In a simple cubic case these three rotations are those that will bring the specimen coordinate system onto the crystal coordinate system:
-1- rotation around Z_S: to bring RD (X_S) into X_C-Y_C plane,
-2- rotation around X'_S: to bring TD (Y'_S) into X_C-Y_C plane, and ND (Z'_S) parallel to Z_C, and
-3- rotation around Z'_S: to bring RD (X'_S) and TD (Y''_S) parallel to X_C and Y_C with ND (Z'_S) parallel to (Z_C).

The rotations for Bunge's Euler angles (default) are shown on the left.

The Roe and Kocks Euler angles are similar. The relationship between these angles is as follows:

Bunge: ($\varphi_1, \Phi, \varphi_2$)
Roe: (Ψ, Θ, Φ) $= (\varphi_1 - 90°, \Phi, 90° - \varphi_2)$
Kocks: (Φ, Θ, ϕ) $= (\varphi_1 - 90°, \Phi, 90° + \varphi_2)$

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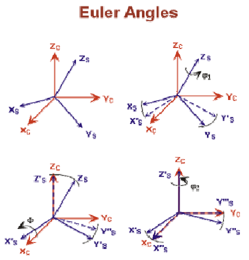
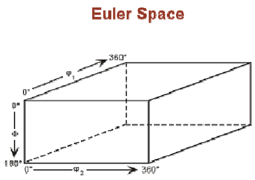
Euler angles

PASSIVE: Orientations are defined as the rotation(s) needed to bring the sample reference frame into coincidence with the crystal reference frame. This is the definition used by Bunge which is used in OIM.
ACTIVE: Orientations are defined as the rotation(s) needed to bring the crystal reference frame into coincidence with the sample reference frame.





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Orthonormal transformations

Transformations (M) from the crystal basis to the orthonormal basis:

$P = [1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2 \cos\alpha \cos\beta \cos\gamma]^{1/2}$

$(xyz) = \mathrm{M}\ (hkl)$

$$\begin{bmatrix} \dfrac{1}{a \sin\beta} & 0 & \dfrac{-\cos\beta}{c \sin\beta} \\ \dfrac{\cos\alpha\cos\beta - \cos\gamma}{a P \sin\beta} & \dfrac{\sin\beta}{bP} & \dfrac{\cos\beta\cos\gamma - \cos\alpha}{c P \sin\beta} \\ 0 & 0 & \dfrac{1}{c} \end{bmatrix}$$

$(hkl) = \mathrm{M}\ (xyz)$

$$\begin{bmatrix} a \sin\beta & 0 & a \cos\beta \\ \dfrac{a(\cos\gamma - \cos\alpha\cos\beta)}{\sin\beta} & \dfrac{bP}{\sin\beta} & b\cos\alpha \\ 0 & 0 & c \end{bmatrix}$$

$(xyz) = \mathrm{M}\ [uvw]$

$$\begin{bmatrix} a \sin\beta & \dfrac{b(\cos\gamma - \cos\alpha\cos\beta)}{\sin\beta} & 0 \\ 0 & \dfrac{bP}{\sin\beta} & 0 \\ a\cos\beta & b\cos\alpha & c \end{bmatrix}$$

If using Miller-Bravais Indices ([u'v't'w'] i.e. for hexagonal or trigonal symmetry) then

$u = 2u' + v'$
$v = 2v' + u'$
$w = w'$

$[uvw] = \mathrm{M}\ (xyz)$

$$\begin{bmatrix} \dfrac{1}{a \sin\beta} & \dfrac{\cos\alpha\cos\beta - \cos\gamma}{a P \sin\beta} & 0 \\ 0 & \dfrac{\sin\beta}{bP} & 0 \\ \dfrac{-\cos\beta}{c\sin\beta} & \dfrac{\cos\beta\cos\gamma - \cos\alpha}{c \sin\beta} & \dfrac{1}{c} \end{bmatrix}$$

If using Miller-Bravais Indices ([u'v't'w'] i.e. for hexagonal or trigonal symmetry) then

$u' = (2u - v)/3$
$v' = (2v - u)/3$
$w' = w$

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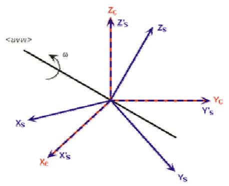
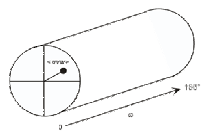
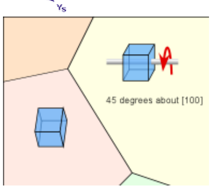
Axis-angle pair

Axis/Angle Definition



Axis/Angle Space





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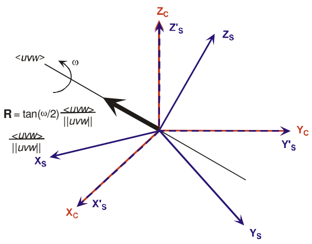
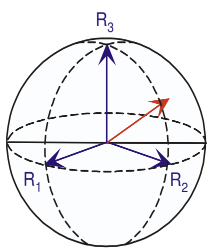
Rodrigues vector

Rodrigues vector definition



Rodrigues space



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Conversions

Euler Angles

Bunge: $(\varphi_1, \Phi, \varphi_2)$

Roe: (Ψ, Θ, Φ) $(\varphi_1 - 90°, \Phi, 90° - \varphi_2)$

Kocks: (Φ, Θ, ϕ) $(\varphi_1 - 90°, \Phi, 90° + \varphi_2)$

Matrix

$$\mathbf{g} = \begin{bmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_2\sin\Phi \\ -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\varphi_2\cos\Phi & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\varphi_2\cos\Phi & \cos\varphi_2\sin\Phi \\ \sin\varphi_1\sin\Phi & -\cos\varphi_1\sin\Phi & \cos\Phi \end{bmatrix}$$

Axis Angle

ω rotation about the axis $\mathbf{d} = [d_1, d_2, d_3]$

$$\mathbf{g} = \begin{bmatrix} (1-d_1^2)\cos\omega + d_1^2 & d_1d_2(1-\cos\omega) + d_3\sin\omega & d_1d_3(1-\cos\omega) - d_2\sin\omega \\ d_1d_2(1-\cos\omega) - d_3\sin\omega & (1-d_2^2)\cos\omega + d_2^2 & d_2d_3(1-\cos\omega) + d_1\sin\omega \\ d_1d_3(1-\cos\omega) + d_2\sin\omega & d_2d_3(1-\cos\omega) - d_1\sin\omega & (1-d_3^2)\cos\omega + d_3^2 \end{bmatrix}$$

$$2\cos\omega = \mathrm{Trace}(\mathbf{g}) - 1 = g_{11} + g_{22} + g_{33} - 1$$

Rodrigues Vector

$$\mathbf{R} = \mathbf{d}\tan\frac{\omega}{2} \quad \text{where} \quad |\mathbf{d}| = \sqrt{d_1^2 + d_2^2 + d_3^2} = 1$$

(hkl)[uvw]

$$h = n\sin\varphi_2\sin\Phi = m(g_{23} - g_{32})$$

$$k = n\cos\varphi_2\sin\Phi = m(g_{13} - g_{31})$$

$$l = n\cos\Phi = m(g_{21} - g_{12})$$

$$u = n'(\cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2\cos\Phi)$$

$$v = n'(-\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\varphi_2\cos\Phi)$$

$$w = n'\sin\varphi_1\sin\Phi$$

$$\cos\Phi = \frac{l}{\sqrt{h^2 + k^2 + l^2}}$$

$$\cos\varphi_2 = \frac{k}{\sqrt{h^2 + k^2}}$$

$$\sin\varphi_2 = \frac{h}{\sqrt{h^2 + k^2}}$$

$$\sin\varphi_1 = \frac{w}{\sqrt{u^2 + v^2 + w^2}}\sqrt{\frac{h^2 + k^2 + l^2}{h^2 + k^2}}$$

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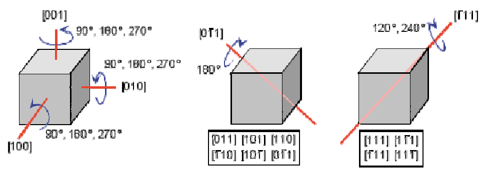
Crystal symmetry

Crystal symmetry: The set of rotations (a point group) which when applied to the crystal lattice rotate the lattice into an orientation indistinguishable from the original orientation. For example consider the symmetries of a cube:



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Crystal symmetry

Mathematically if an orientation is represented as a matrix then the symmetry elements of the point group can be represented as a set of matrices (L_i):

$\mathbf{L}_1 = E = \begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}$	$\mathbf{L}_7 = L^3_{\bar{1}1\bar{1}} = \begin{bmatrix}0&-1&0\\0&0&-1\\1&0&0\end{bmatrix}$	$\mathbf{L}_{13} = L^2_{10\bar{1}} = \begin{bmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{bmatrix}$	$\mathbf{L}_{19} = L^2_{011} = \begin{bmatrix}1&0&0\\0&0&1\\0&-1&0\end{bmatrix}$
$\mathbf{L}_2 = L^2_{010} = \begin{bmatrix}-1&0&0\\0&1&0\\0&0&-1\end{bmatrix}$	$\mathbf{L}_8 = L^3_{\bar{1}\bar{1}1} = \begin{bmatrix}0&1&0\\0&0&-1\\-1&0&0\end{bmatrix}$	$\mathbf{L}_{14} = L^2_{101} = \begin{bmatrix}0&0&1\\0&-1&0\\1&0&0\end{bmatrix}$	$\mathbf{L}_{20} = L^2_{011} = \begin{bmatrix}-1&0&0\\0&0&1\\0&1&0\end{bmatrix}$
$\mathbf{L}_3 = L^2_{001} = \begin{bmatrix}-1&0&0\\0&-1&0\\0&0&1\end{bmatrix}$	$\mathbf{L}_9 = L^3_{\bar{1}\bar{1}\bar{1}} = \begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}$	$\mathbf{L}_{15} = L^4_{0\bar{1}0} = \begin{bmatrix}0&0&1\\0&1&0\\-1&0&0\end{bmatrix}$	$\mathbf{L}_{21} = L^2_{\bar{1}10} = \begin{bmatrix}0&-1&0\\-1&0&0\\0&0&-1\end{bmatrix}$
$\mathbf{L}_{10} = L^3_{11\bar{1}} = \begin{bmatrix}0&0&-1\\1&0&0\\0&-1&0\end{bmatrix}$	$\mathbf{L}_4 = L^2_{100} = \begin{bmatrix}1&0&0\\0&-1&0\\0&0&-1\end{bmatrix}$	$\mathbf{L}_{16} = L^4_{010} = \begin{bmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{bmatrix}$	$\mathbf{L}_{22} = L^4_{001} = \begin{bmatrix}0&1&0\\-1&0&0\\0&0&1\end{bmatrix}$
$\mathbf{L}_5 = L^3_{111} = \begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}$	$\mathbf{L}_{11} = L^3_{\bar{1}11} = \begin{bmatrix}0&0&-1\\-1&0&0\\0&1&0\end{bmatrix}$	$\mathbf{L}_{17} = L^2_{01\bar{1}} = \begin{bmatrix}-1&0&0\\0&0&-1\\0&-1&0\end{bmatrix}$	$\mathbf{L}_{23} = L^2_{110} = \begin{bmatrix}0&1&0\\1&0&0\\0&0&-1\end{bmatrix}$
$\mathbf{L}_6 = L^3_{1\bar{1}\bar{1}} = \begin{bmatrix}0&-1&0\\0&0&1\\-1&0&0\end{bmatrix}$	$\mathbf{L}_{12} = L^3_{1\bar{1}1} = \begin{bmatrix}0&0&1\\-1&0&0\\0&-1&0\end{bmatrix}$	$\mathbf{L}_{18} = L^4_{100} = \begin{bmatrix}1&0&0\\0&0&-1\\0&1&0\end{bmatrix}$	$\mathbf{L}_{24} = L^4_{00\bar{1}} = \begin{bmatrix}0&-1&0\\1&0&0\\0&0&1\end{bmatrix}$

The mathematical relation can then be written as: $g^e = L_i g$ where g^e is an orientation symmetrically equivalent to the original orientation, g. For misorientations the relation is given as follows:

$$\Delta\mathbf{g} = \mathbf{g}_B\mathbf{g}_A^T$$

$$\Delta\mathbf{g}^e = \mathbf{L}_i\mathbf{g}_B(\mathbf{L}_j\mathbf{g}_A)^T$$

$$\Delta\mathbf{g}^e = \mathbf{L}_i\mathbf{g}_B(\mathbf{g}_A^T\mathbf{L}_j^T) \quad \text{but } \mathbf{L}_j^T \text{ is a member of the symmetry point group}$$

$$\Delta\mathbf{g}^e = \mathbf{L}_i\Delta\mathbf{g}\mathbf{L}_k$$

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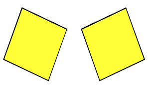
Sample symmetry

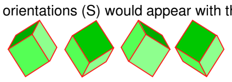
Sample symmetry: Sample symmetry arises from symmetry in the material processing. It is sometimes referred to as statistical symmetry. Consider for example the rolling of sheet metals. This forming operation has orthotropic symmetry. Mathematically if an orientation is represented as a matrix then the symmetry elements of the point group can be represented as a set of matrices ($\mathbf{R}_i$):

$\mathbf{R}_1 = E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\mathbf{R}_3 = L^2_{010} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
$\mathbf{R}_2 = L^2_{001} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\mathbf{R}_4 = L^2_{100} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$

The term statistical symmetry is probably most accurate as what is implied by sample symmetry is that there are statistically as many grains in one orientation as in a symmetrically equivalent one.
For example the following orientations (in 2-d) would appear with the same frequency:



In 3D the following orientations (S) would appear with the same frequency in rolled sheet:



The mathematical relation can then be written as: $\mathbf{g}^e = \mathbf{g}\,\mathbf{R}_i$ where $\mathbf{g}^e$ is an orientation symmetrically equivalent to the original orientation, $\mathbf{g}$

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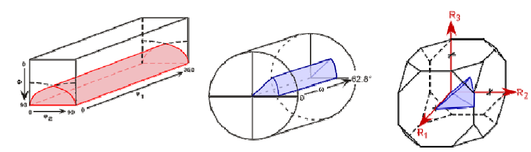
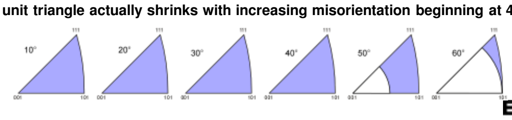
Fundamental region

Because of symmetry the orientation space can be reduced to a fundamental region or asymmetric domain containing only unique orientations (i.e. no symmetrically equivalent orientations). The following examples are for cubic crystal symmetry.



***The unit triangle actually shrinks with increasing misorientation beginning at 45°.**



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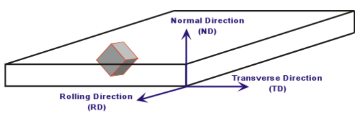
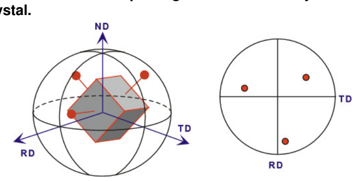
Pole figures

Consider a cubic crystal in a rolled sheet sample with "laboratory" or "sample" axes as shown below.



The Pole figure plots the orientation of a given lattice plane normal (pole) with respect to the sample reference frame. The example below is a (001) pole figure. Note the three points shown in the pole figure are for three symmetrically equivalent planes in the crystal.



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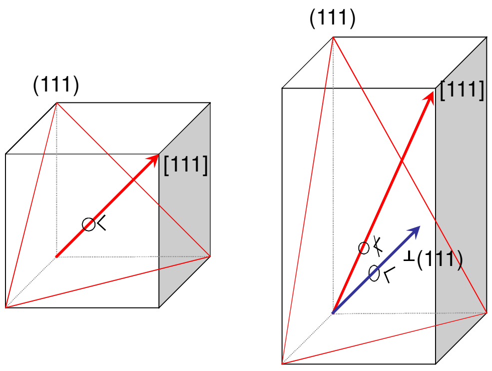
Planes, poles, and directions



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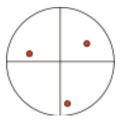
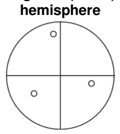
Pole figures: negative hemisphere

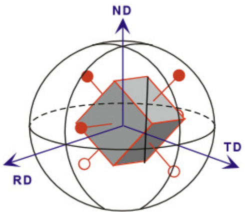
Open circles can be used to distinguish points in the negative hemisphere from points in the positive hemisphere in the same pole figure.

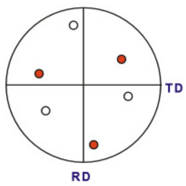


Positive (upper) hemisphere

Negative (lower) hemisphere







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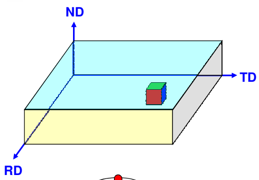
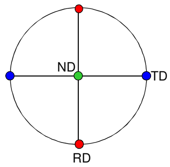
Pole figures – single orientation

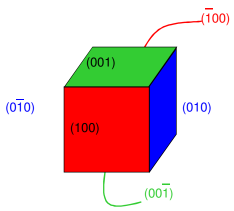


A pole figure shows the orientation of a given plane normal (a “pole”) with respect to the sample axes.



(001) Pole figure

(should actually be written as {001} because all symmetric equivalents are included)



{100} planes in a cubic crystal

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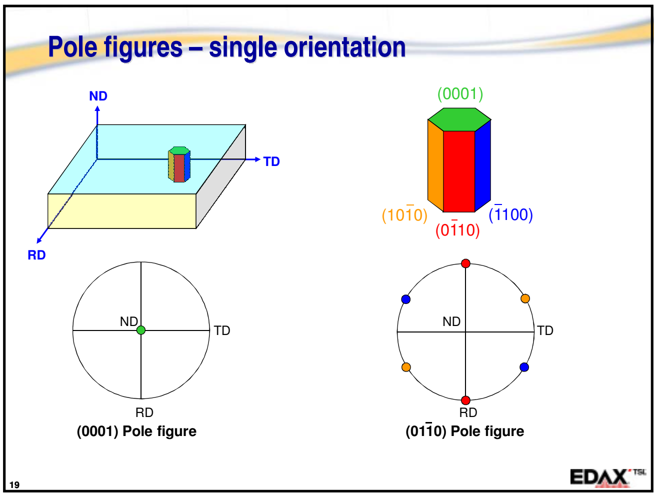
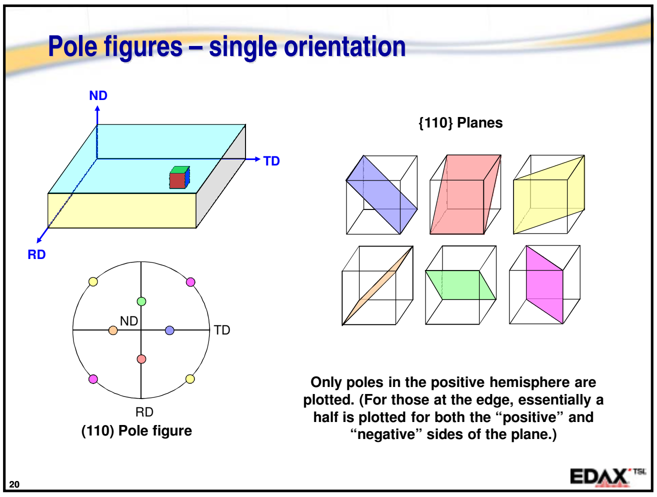
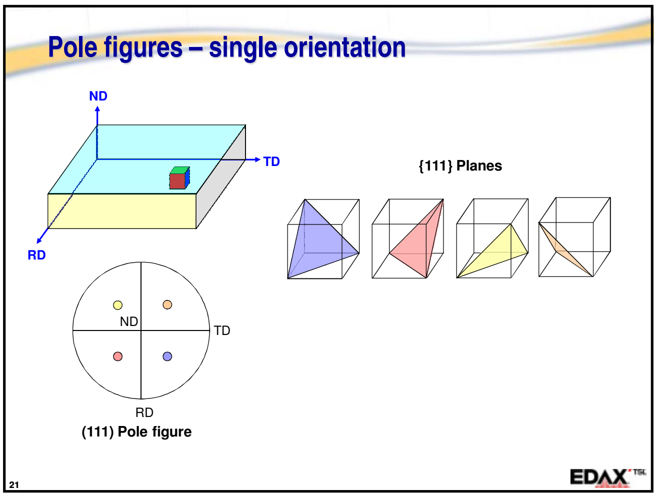
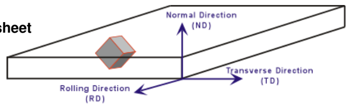

Pole figures – single orientation
ND
TD
RD
(0001)
$(10\bar{1}0)$
$(01\bar{1}0)$
$(\bar{1}100)$
ND
TD
RD
(0001) Pole figure
ND
TD
RD
$(01\bar{1}0)$ Pole figure
19
EDAX


Pole figures – single orientation
ND
TD
RD
{110} Planes
ND
TD
RD
(110) Pole figure
Only poles in the positive hemisphere are plotted. (For those at the edge, essentially a half is plotted for both the "positive" and "negative" sides of the plane.)
20
EDAX


Pole figures – single orientation
ND
TD
RD
{111} Planes
ND
TD
RD
(111) Pole figure
21
EDAX

Inverse pole figures

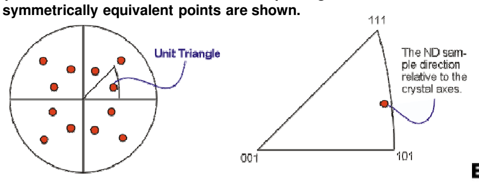
Consider a cubic crystal in a rolled sheet sample with "laboratory" or "sample axes as shown.



The Inverse Pole Figure plots the orientation of a given specimen direction (typically the sample normal) with respect to the crystal axes.

There are two ways of looking at inverse pole figures:
1) Which crystal axis is aligned with a specified sample axis.
2) The orientation of the specified sample axis with respect to the crystal axes.

The example below is a normal direction inverse pole figure. In the full inverse pole figure all symmetrically equivalent points are shown.



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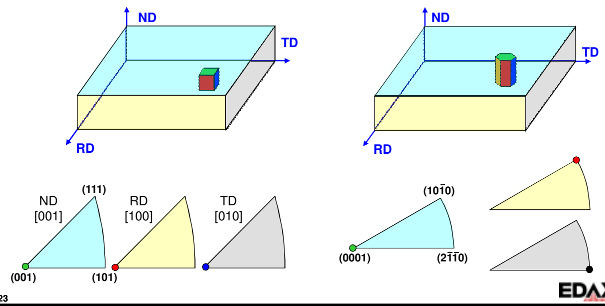
Inverse pole figures – single orientation

An inverse pole figure shows the pole that is parallel to a given sample direction

Because of crystal symmetry only a “unit triangle” is needed instead of a full circle. The triangle changes from symmetry to symmetry



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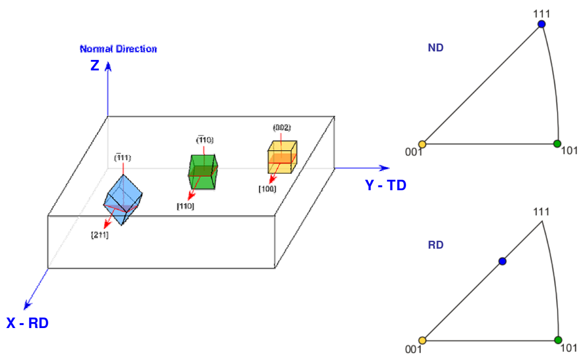
Inverse pole figures



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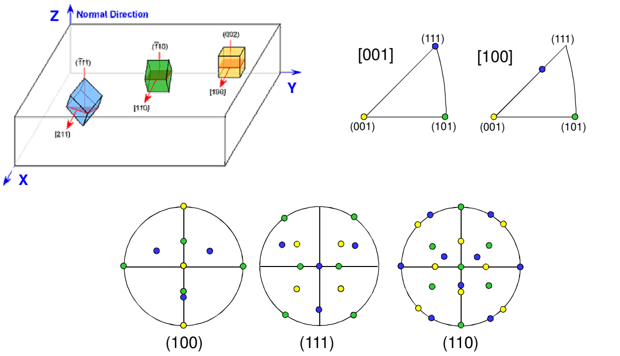
Comparison – three orientations



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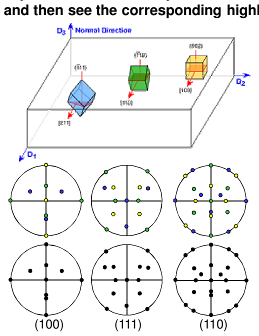
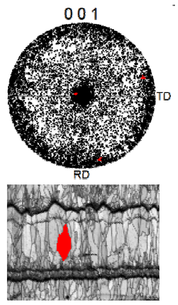
Comparison – three orientations

But in typical analysis of EBSD data, all points are shown in a single color so you can't tell which points should be grouped together. However, one of the powerful capabilities of OIM Analysis is the ability to highlight individual grains in a map and then see the corresponding highlighting in the pole figure.





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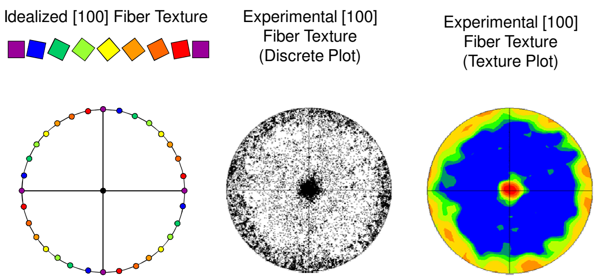
Set of orientations



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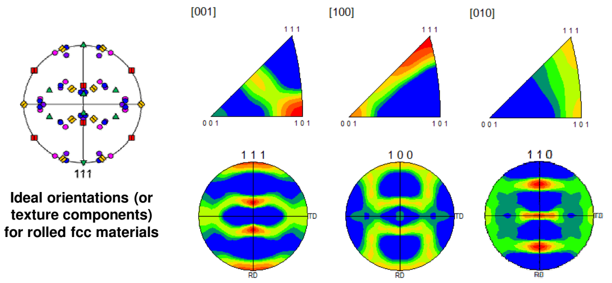
Rolling texture

Other textures can be much more complicated such as a rolling texture. The following is an example for rolled copper. Note the peak at (110) in the normal direction inverse pole figure and the peak at (111) in the reference direction inverse pole figure. This suggests that the (110)[111] orientation is an important one in this material.



Ideal orientations (or texture components) for rolled fcc materials

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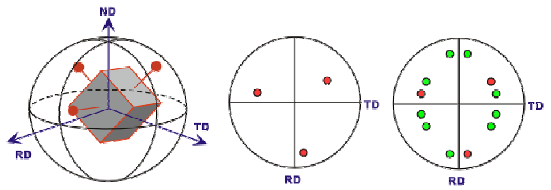
Pole figures: crystal & sample symmetry



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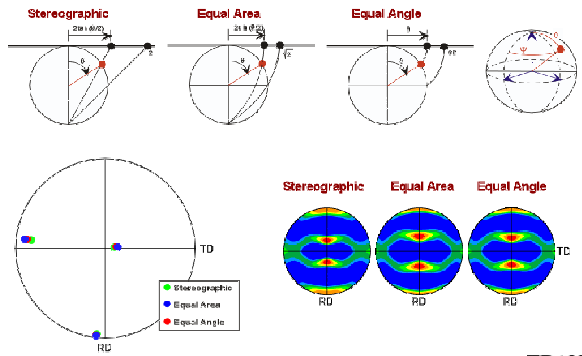
Projections



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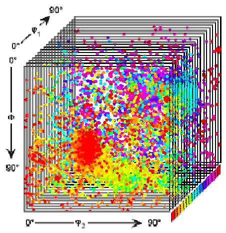
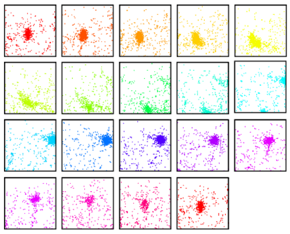
Euler space sections





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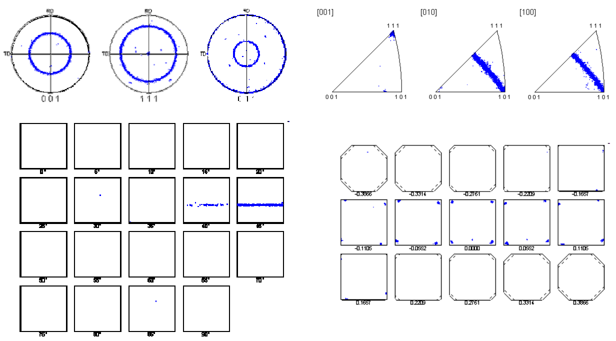
Comparison



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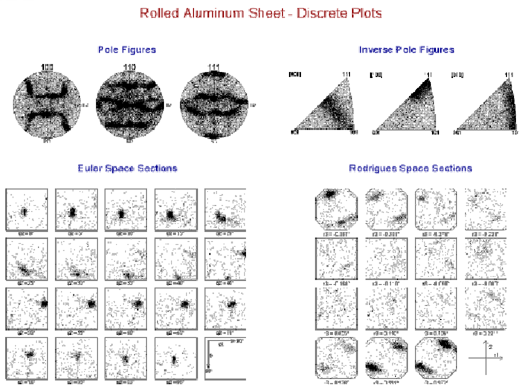
Comparison



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References

For a description of the representation of orientation, especially in terms of Euler angles, and the mathematics behind the harmonic expansion of the ODF see:

H. Bunge (1982). *Texture Analysis in Materials Science*. Butterworths: London.

For a general overview of textures in metals see:

I. Dillamore and W. Roberts (1965). Preferred orientation in Wrought and Annealed Metals. *Metallurgical Reviews* 10, 271-380

For a general overview of textures in hexagonal materials see the first few chapters of:

E. Tenckhoff (1988). *Deformation Mechanisms, Texture and Anisotropy in Zirconium and Zircaloy.* ASTM: Philadelphia.

A good place to become familiar with the general body of literature in texture analysis is in the proceedings of the International Conference on Texture of Materials (ICOTOM) held every three years.

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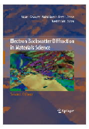

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