Crystal Geometry

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MTEX Workshop 2019

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Three dimensional vectors - The MTEX Class **vector3d**

Three dimensional vectors are given by there coordinates with respect to a orthogonal coordinate system $\vec{X}, \vec{Y}, \vec{Z}$

$$\vec{r} = x \cdot \vec{X} + y \cdot \vec{Y} + z \cdot \vec{Z}$$

For general vectors, MTEX does **not** care about the coordinate system, but works only with the coordinates.

```
r = vector3d(1,2,3)
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```
r = vector3d (show methods, plot)
  size: 1 x 1
  x y z
  1 2 3
```

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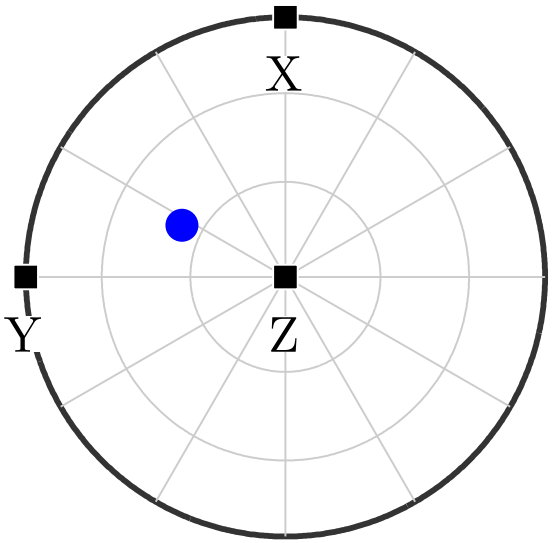
```
r = vector3d(1,2,3)
```

The alignment of the coordinate system is only important when plotting data

```
plotx2north, plotzOutOfPlane
plot(r)
```



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```
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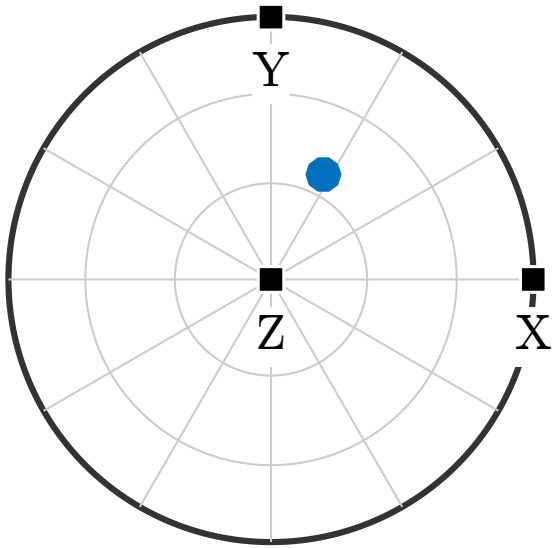

Only for directions relative to the crystal coordinate system the reference frame is considered.

Defining vectors

polar coordinates $\vec{r} = (\sin\theta\cos\rho, \sin\theta\sin\rho, \cos\theta)^t$

```
theta = 90 * degree; rho = 45 * degree;
r = vector3d.byPolar(theta,rho)
```

In MTEX all angles are in radiant!

predefined vectors

```
vector3d.X, vector3d.Y, vector3d.Z
```

combine vectors

```
r = [vector3d.X, vector3d.Y, vector3d(1,1,1)];
```

importing vectors

```
r = vector3d.load('file','ColumnNames',{'x','y','z'})
```

random vectors

```
r = vector3d.rand(100)
```

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  x y z
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r = vector3d.load('file','ColumnNames',{'x','y','z'})
```

```
r = vector3d (show methods, plot)
  size: 200 x 1
```

random vectors

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theta = 90 * degree; rho = 45 * degree;
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Vector Calculations

simple algebra

```
r = 2*vector3d.X - vector3d.Y;
```

basic operations

```
dot(v1,v2)    % dot product
cross(v1,v2)  % cross product
angle(v1,v2)  % angle between two vectors
```

density estimation

```
sF = calcDensity(v,'halfwidth',5*degree)
```

extract properties

```
r.theta       % polar angle in radiant
r.rho         % azimuth angle in radiant
r.x, r.y, r.z
```

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density estimation

```
sF = calcDensity(v,'halfwidth',5*degree)
```

```
sF = S2FunHarmonic (show methods, plot)
 bandwidth: 25
```

extract properties

```
r.theta      % polar angle in radiant
r.rho        % azimuth angle in radiant
r.x, r.y, r.z
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Vector Calculations

simple algebra

```
r = 2*vector3d.X - vector3d.Y;
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r.theta       % polar angle in radiant
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r.x, r.y, r.z
```

Indexing of Vectors

consider a list of vectors

```
r = vector3d([0 0 1 1],[1 0 1 1],[1 1 1 0]);
```

```
r = vector3d (show methods, plot)
  size: 1 x 4
  x y z
  0 1 1
  0 0 1
  1 1 1
  1 1 0
```

single out the second vector

```
r(2)
```

single out the second and the fourth vector

```
r([2 4])
```

single out vectors by a logical condition

```
r(r.x>0)
```

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The above techniques applies also to lists of rotations, orientations,

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single out vectors by a logical condition

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r(r.x>0)
```

The above techniques applies also to lists of rotations, orientations, tensors, EBSD data, grains, boundary segments, triple points, etc.

Changing Vectors

consider again the list of vectors

```
r = vector3d([0 0 1 1],[1 0 1 1],[1 1 1 0]);
```

```
r = vector3d (show methods, plot)
  size: 1 x 4
  x y z
  0 1 1
  0 0 1
  1 1 1
  1 1 0
```

replace the second vector by another vector

```
r(2) = vector3d.Y
```

remove the second vector completely

```
r(2) = []
```

change the x coordinate of all vectors

```
r.x = 0
```

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remove the second vector completely

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r(2) = []
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```
r = vector3d (show methods, plot)
  size: 1 x 3
  0 1 1
  1 1 1
  1 1 0
```

change the x coordinate of all vectors

```
r.x = 0
```

The above techniques applies also to pole figure data, orientations, EBSD

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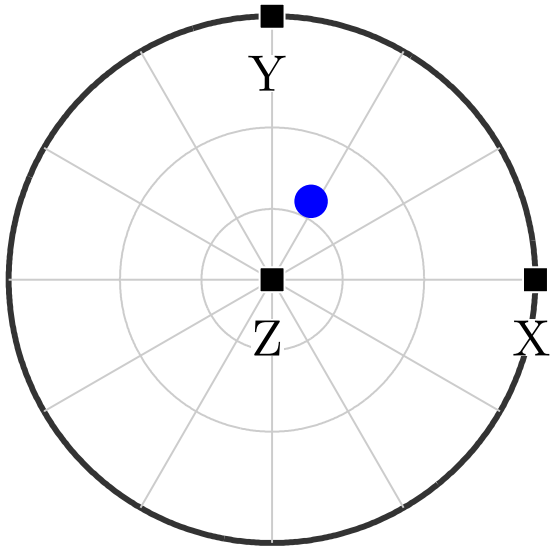
The above techniques applies also to pole figure data, orientations, EBSD data, grains, etc.

Plotting Vectors

spherical projections: `earea`, `edist`, `eangle`

```
plot(r,'projection','eangle','upper')
```



combined plots

```
plot(vector3d(1,1,1),'upper');
hold on
plot(vector3d(1,2,3),'label','B');
plot(vector3d(-1,2,1),'label','A');
hold off
```

scatter plots

```
v = vector3d.rand(1000)
plot(v)
```

contour plots

```
plot(v,'contourf')
```

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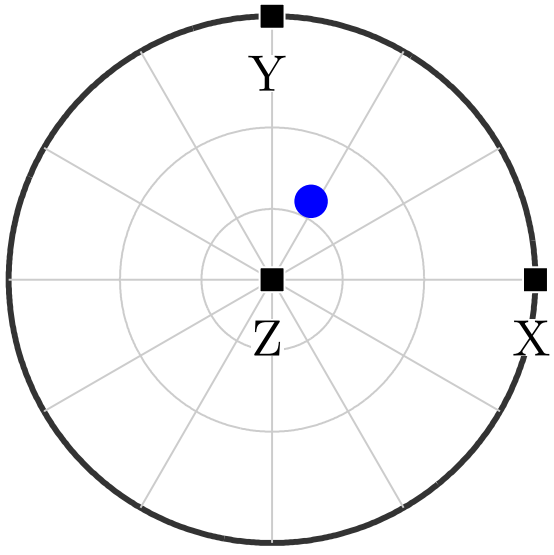

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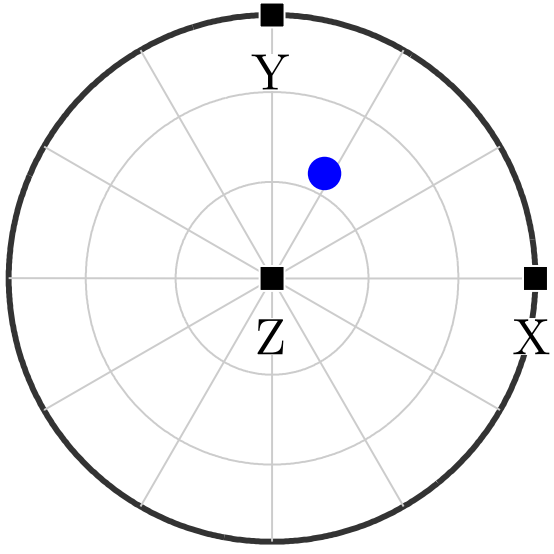

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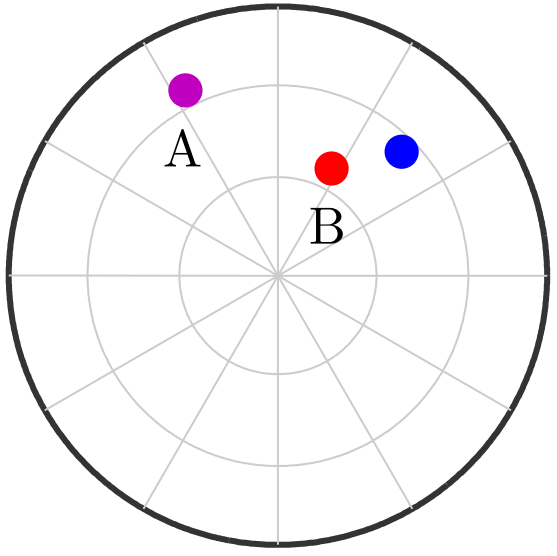

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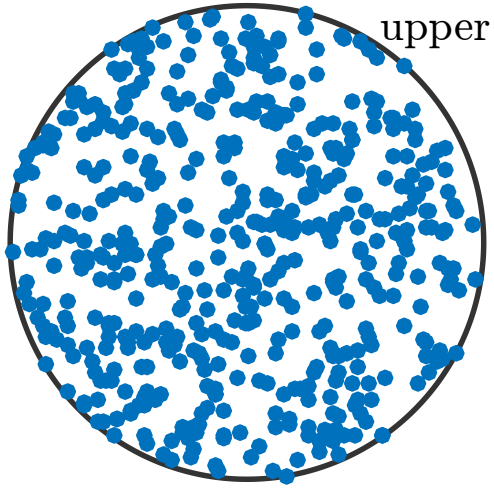

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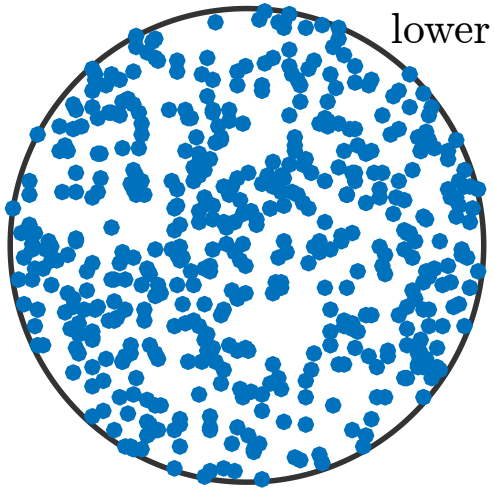

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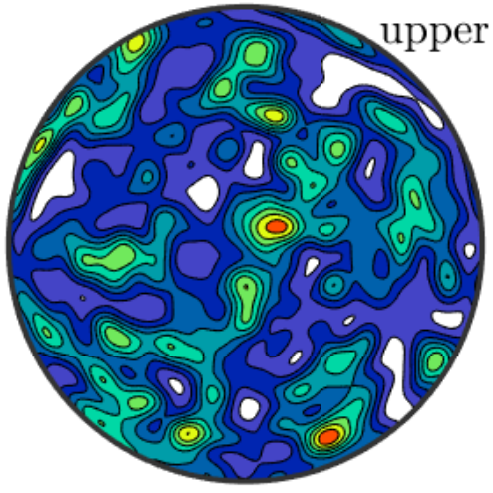

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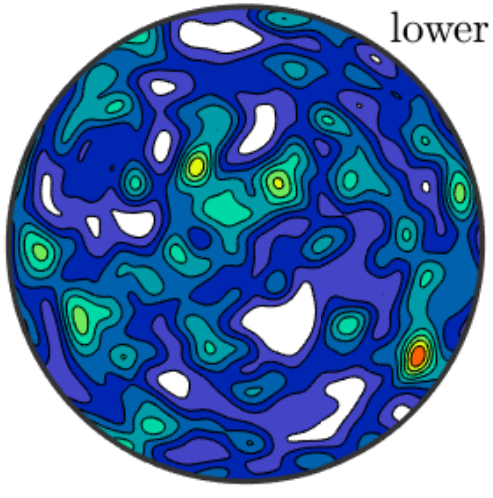

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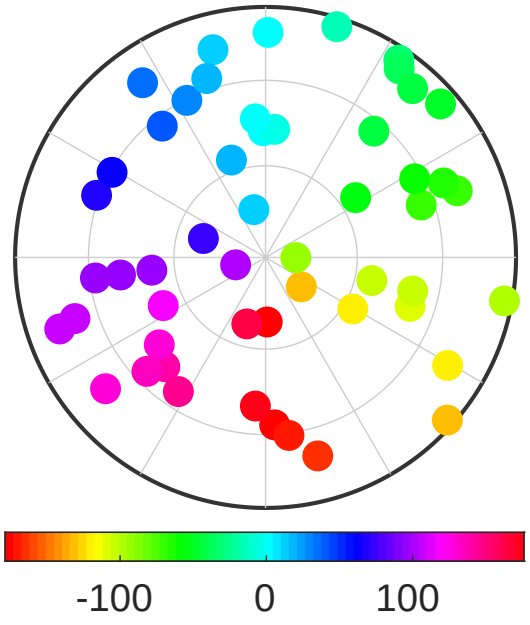
Data Plots

colorize vectors by value

```
v = vector3d.rand(100)
scatter(v,v.rho./degree)
mtexColorbar southoutside
mtexColorMap hsv
```



colorize by RGB triples

```
key = HSVDirectionKey
scatter(v,key.direction2color(v))
```

visualize directions

```
quiver(v,orth(v)) % a vector field
```

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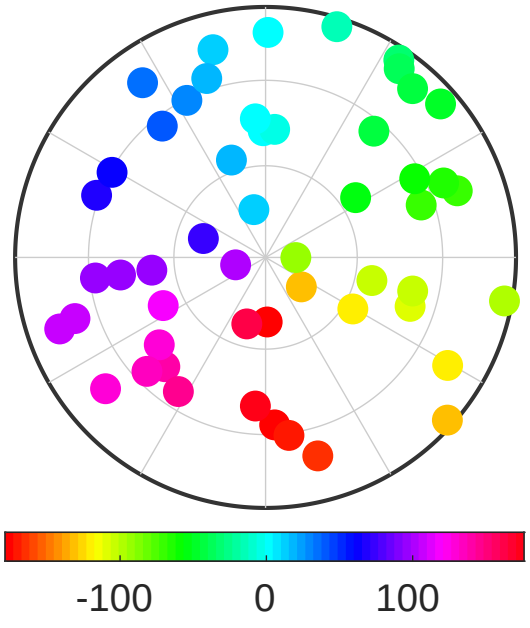

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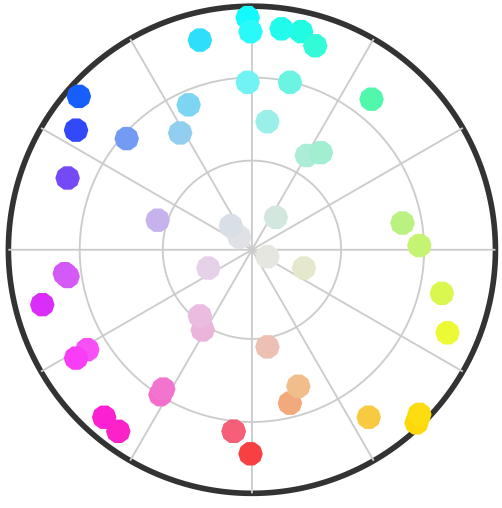

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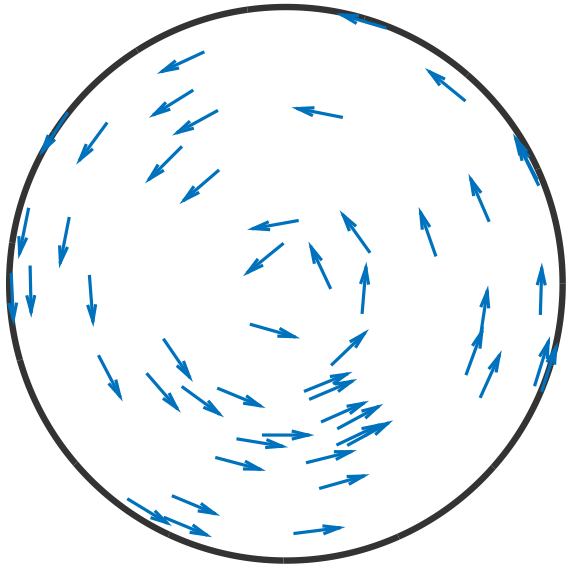

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Axes

Axes are three dimensional vectors where we do not care about length and direction, e.g. plane normals.

```
r = vector3d(1,1,1,'antipodal')
```

```
r = vector3d (show methods, plot)
 size: 1 x 1
 antipodal: true
  x y z
  1 1 1
```

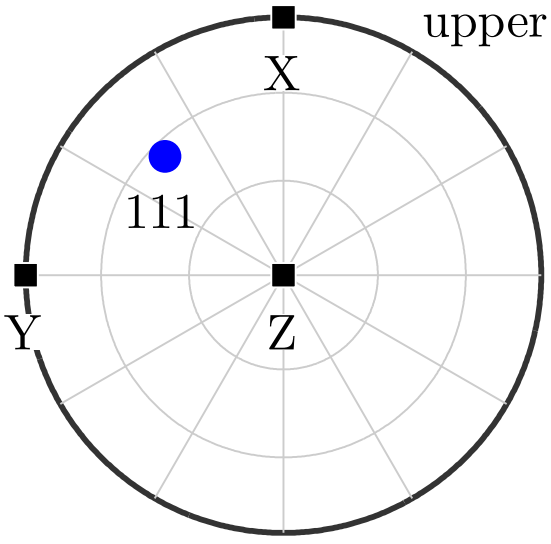
Then `r` and `-r` represent the same axis

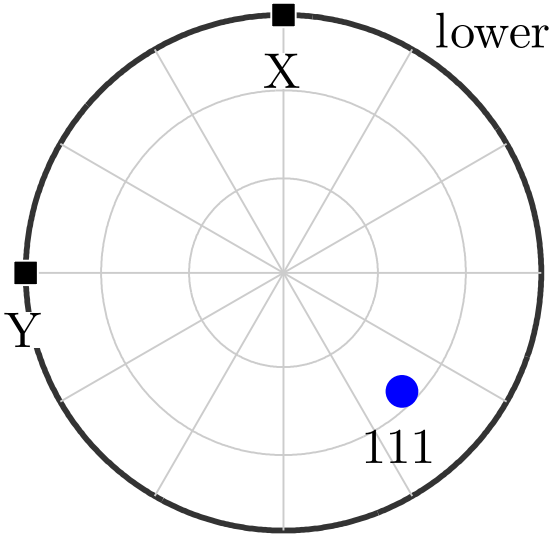
```
eq(r, -r)
```

The angle to an axis is always less then 90°

```
angle(r,-vector3d.X) / degree
```

The option **antipodal** in density estimation





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1
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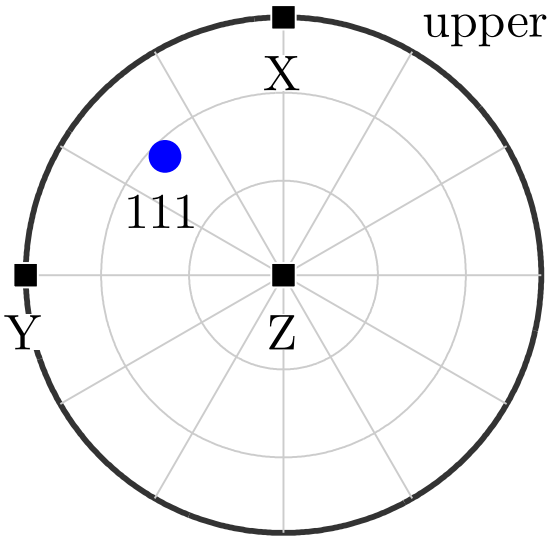

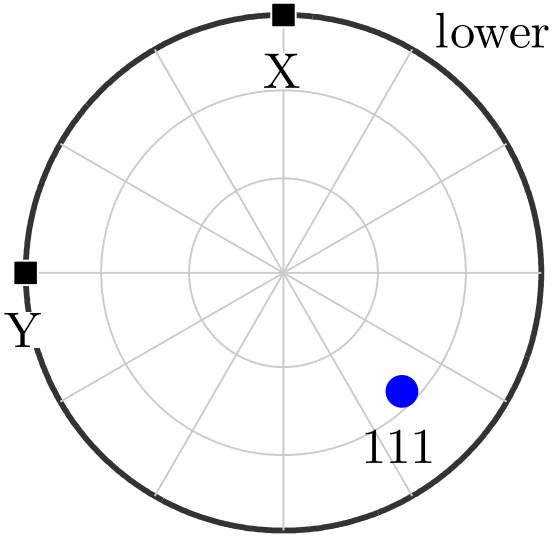

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```

```
  54.7
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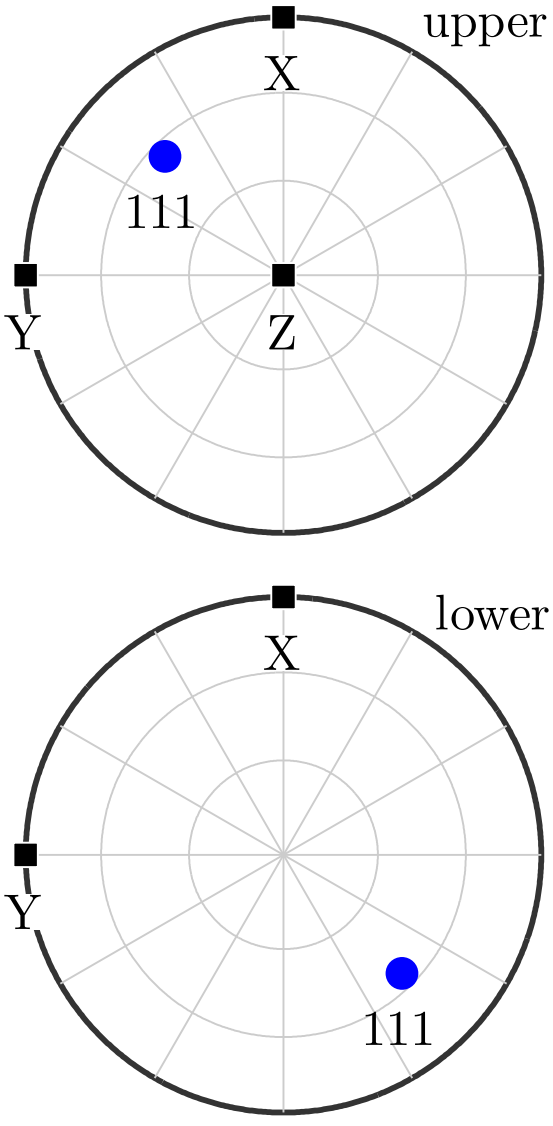


Axes

Axes are three dimensional vectors where we do not care about length and direction, e.g. plane normals.

```
r = vector3d(1,1,1,'antipodal')
```

Then `r` and `-r` represent the same axis

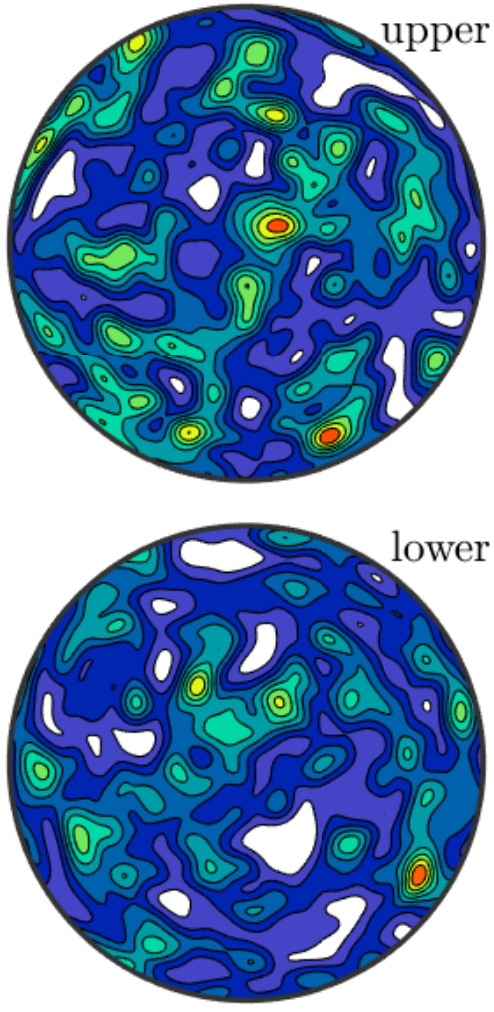
```
eq(r, -r)
```

The angle to an axis is always less then 90°

```
angle(r,-vector3d.X) / degree
```

The option **antipodal** in density estimation

```
r = vector3d.rand(1000)
sF = calcDensity(r)
contourf(sF)
```



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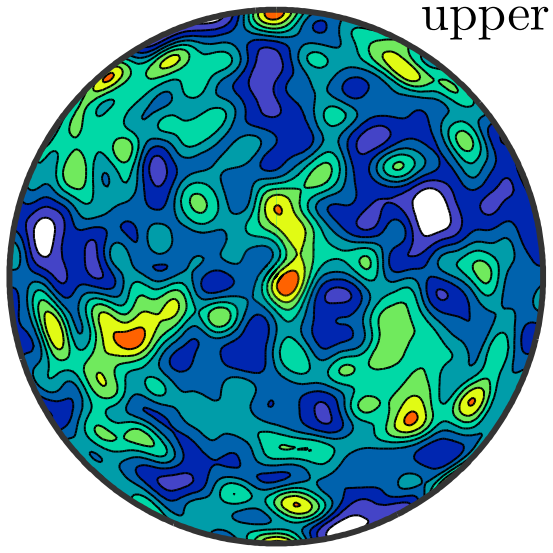

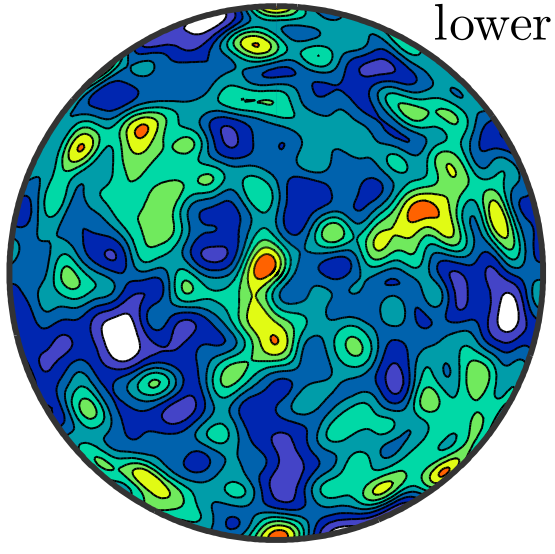

Rotations

A rotation is a transformation that maps a right handed coordinate system $(\vec{X}_1, \vec{Y}_1, \vec{Z}_1)$ onto another right handed coordinate system $(\vec{X}_2, \vec{Y}_2, \vec{Z}_2)$. It is given by the rotation matrix

$$\mathbf{R} = (\vec{X}_2, \vec{Y}_2, \vec{Z}_2) \cdot (\vec{X}_1, \vec{Y}_1, \vec{Z}_1)^t$$

We have $\mathbf{R}\vec{X}_1 = \vec{X}_2$, $\mathbf{R}\vec{Y}_1 = \vec{Y}_2$ and $\mathbf{R}\vec{Z}_1 = \vec{Z}_2$.

On the other hand, $\mathbf{R}$ transforms coordinates with respect to $(\vec{X}_2, \vec{Y}_2, \vec{Z}_2)$ into coordinates with respect to $(\vec{X}_1, \vec{Y}_1, \vec{Z}_1)$. I.e. for

$$\vec{r} = x_1\vec{X}_1 + y_1\vec{Y}_1 + z_1\vec{Z}_1 = x_2\vec{X}_2 + y_2\vec{Y}_2 + z_2\vec{Z}_2$$

we have

$$\mathbf{R}\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$$

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$$\mathbf{R}\begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$$

Euler Angles

Most commonly, rotations are given by Bunge Euler angles.

```
R = rotation.byEuler(10*degree,20*degree,30*degree)
```

```
R = rotation (show methods, plot)
  size: 1 x 1

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
    10    20    30     0
```

```
R = rotation.byEuler(...
    10*degree,20*degree,30*degree,'Roe')
```

Supported conventions are Bunge, Matthies, Roe, Kocks, Canova.

```
setMTEXpref('EulerAngleConvention','Roe')
```

Load orientations from file

```
R = rotation.load(fname,'columns',[2 3 4],...
    'ColumnNames',{'phi1','Phi','phi2'})
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  Roe Euler angles in degree
  Psi  Theta    Phi  Inv.
   10     20     30     0
```

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Other Ways to Define a Rotation

A rotation is uniquely defined by its rotation axis and its rotation angle

```
R = rotation.byAxisAngle(vector3d.X, 45*degree)
```

Conversely, one can compute axis / angle from a rotation

```
R.axis , R.angle
```

Given four vectors $\vec{u}_1, \vec{u}_2, \vec{v}_1, \vec{v}_2$ there is a unique rotation $\mathbf{R}$ such that $\mathbf{R}\vec{u}_1 = \vec{v}_1$ and $\mathbf{R}\vec{u}_2 = \vec{v}_2$

```
R = rotation.map(u1, v1, u2, v2)
```

Of course one can also define a rotation by its 3×3 matrix

```
R = rotation.byMatrix(A)
```

or by quaternions

```
R = rotation(quaternion(a, b, c, d))
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```

Basic Calculations

rotate a vector

```
R = rotation.byAxisAngle(vector3d.X,-45*degree);
R * vector3d(0,1,1)
```

```
ans = vector3d (show methods, plot)
  size: 1 x 1
  x         y         z
  0 1.41421         0
```

the inverse rotation

```
inv(R)
```

combine rotations

```
R * inv(R)
```

plotting

```
R = rotation.rand(100)
scatter(R,R.angle)
```

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```
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  size: 1 x 1

  Bunge Euler angles in degree
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     0    45     0     0
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R = rotation.rand(100)
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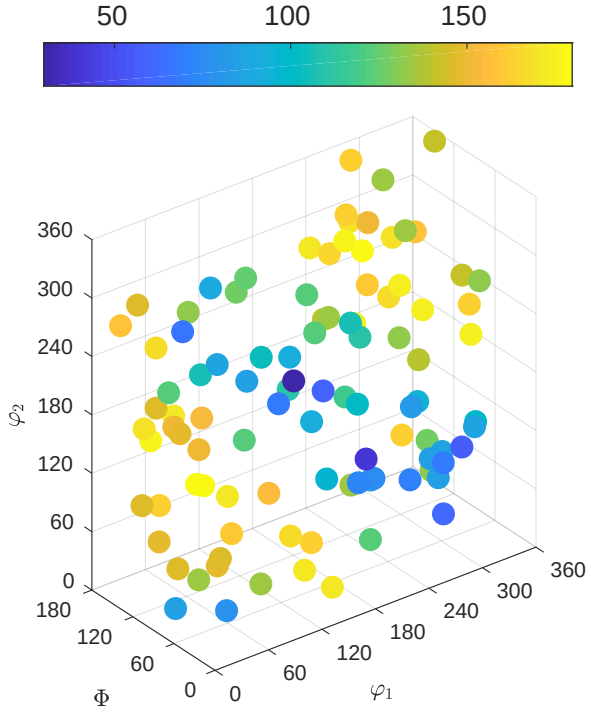
```

```
scatter(R,R.angle,'axisAngle')
```



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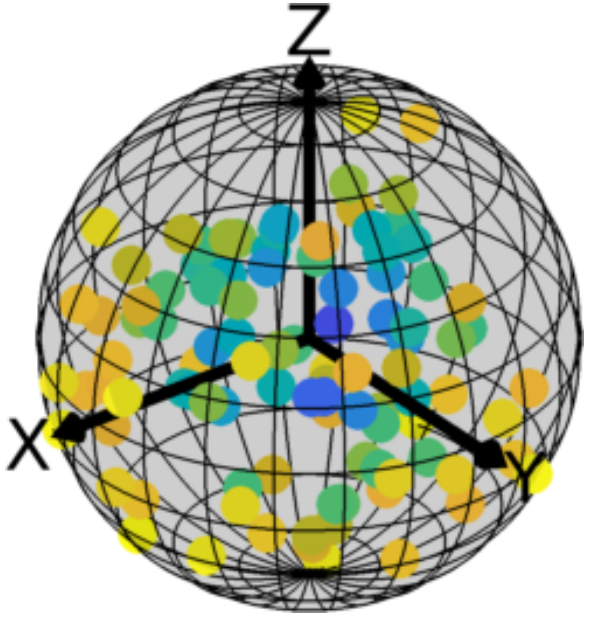

Improper Rotations

an improper rotation is a rotation followed by an inversion

```
I = -rotation.byEuler(10*degree,20*degree,30*degree)
```

```
I = rotation (show methods, plot)
  size: 1 x 1

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
    10    20    30     1
```

reflections

```
R = reflection(vector3d.X + vector3d.Y)
```

angles between proper and improper rotations

```
angle(I,[R,-R])
```

check for improper rotations

Improper Rotations

an improper rotation is a rotation followed by an inversion

```
I = -rotation.byEuler(10*degree,20*degree,30*degree)
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```
R = rotation (show methods, plot)
  size: 1 x 1

  Bunge Euler angles in degree
  phi1  Phi phi2 Inv.
    45  180  315    1
```

angles between proper and improper rotations

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angle(I,[R,-R])
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Improper Rotations

an improper rotation is a rotation followed by an inversion

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R = reflection(vector3d.X + vector3d.Y)
```

angles between proper and improper rotations

```
angle(I,[R,-R])
```

```
  168.5677  180.0000
```

check for improper rotations

```
I.isImproper
```

Improper Rotations

an improper rotation is a rotation followed by an inversion

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I = -rotation.byEuler(10*degree,20*degree,30*degree)
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check for improper rotations

```
I.isImproper
```

```
  1
```

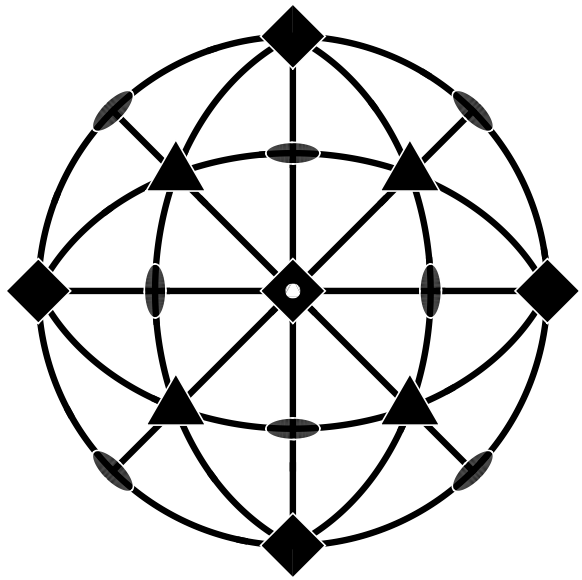
Crystal Symmetry

The point group **C** of a crystal are all rotations **R** that keep the crystal lattice invariant.

```
CS = crystalSymmetry('m-3m')
```

```
CS = crystalSymmetry (show methods, plot)

  symmetry: m-3m
  a, b, c : 1, 1, 1
```



extract the rotations of a point group

```
rotation(crystalSymmetry('222'))
```

import from crystal information files

```
CS=crystalSymmetry.load('qu.cif')
```

import from phl files

```
CS=crystalSymmetry.load('mag.phl')
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switch to Laue / purely rotational group

Crystal Symmetry

The point group **C** of a crystal are all rotations **R** that keep the crystal lattice invariant.

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CS = crystalSymmetry('m-3m')
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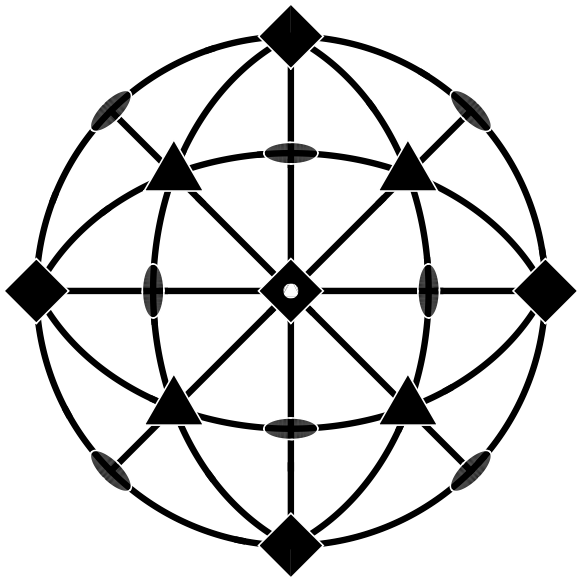

extract the rotations of a point group

```
rotation(crystalSymmetry('222'))
```

```
ans = rotation (show methods, plot)
  size: 4 x 1

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
     0     0     0     0
   180     0     0     0
    45   180    45     0
    45   180   225     0
```

import from crystal information files

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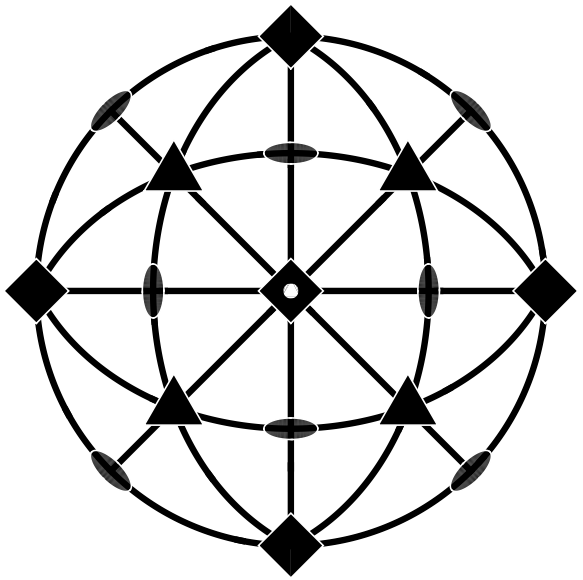


extract the rotations of a point group

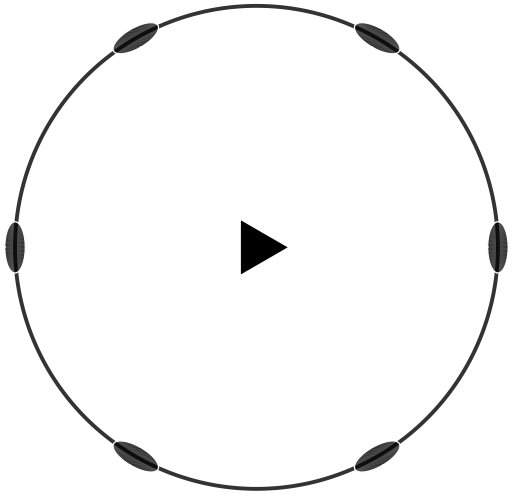
```
rotation(crystalSymmetry('222'))
```

import from crystal information files

```
CS=crystalSymmetry.load('qu.cif')
```

```
CS = crystalSymmetry (show methods, plot)

  mineral              : Quartz
  symmetry             : P 32 2 1 (321)
  a, b, c              : 4.9, 4.9, 5.4
  alpha, beta, gamma   : 90, 90, 120
  reference frame      : X||a*, Y||b, Z||c*
```



import from phl files

```
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```

Crystal Symmetry

The point group **C** of a crystal are all rotations **R** that keep the crystal lattice invariant.

```
CS = crystalSymmetry('m-3m')
```

extract the rotations of a point group

```
rotation(crystalSymmetry('222'))
```

import from crystal information files

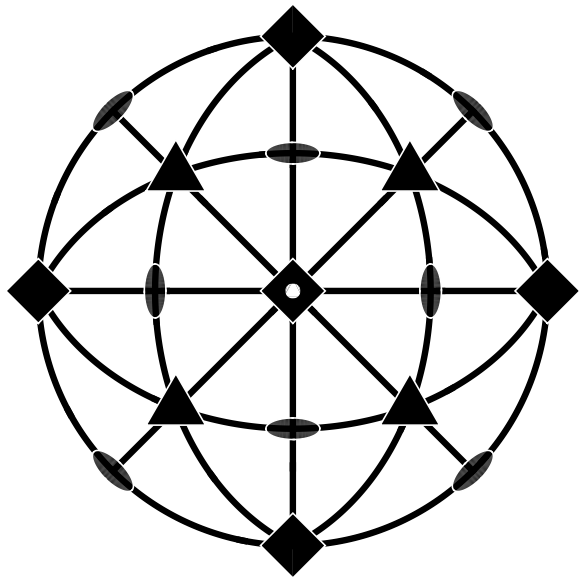
```
CS=crystalSymmetry.load('qu.cif')
```

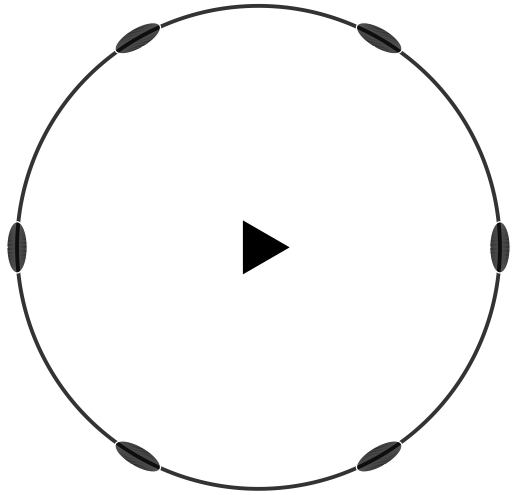
import from phl files

```
CS=crystalSymmetry.load('mag.phl')
```

```
CS{1} = crystalSymmetry (show methods, plot)

  mineral : Magnetite
  density : 5.054
  symmetry: m-3m
  a, b, c : 8.4, 8.4, 8.4
```





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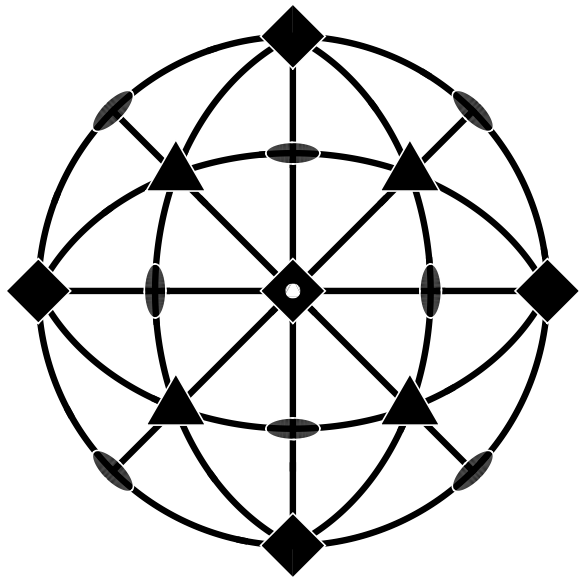
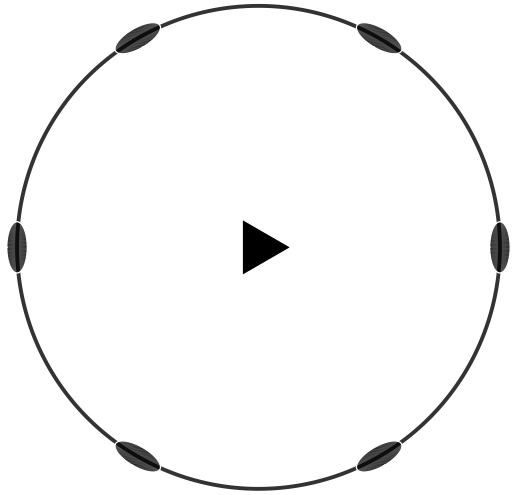
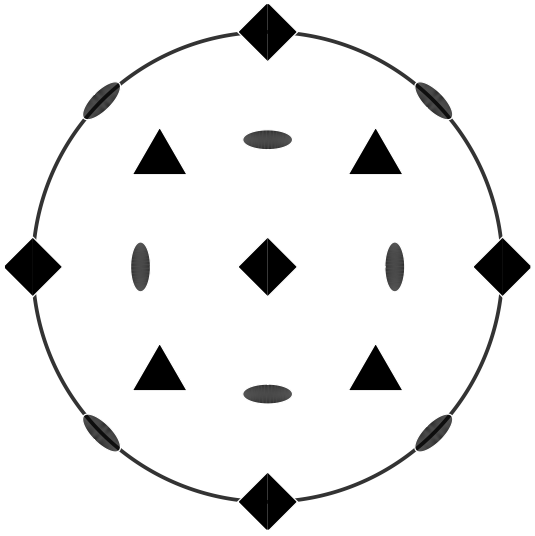
switch to Laue / purely rotational group

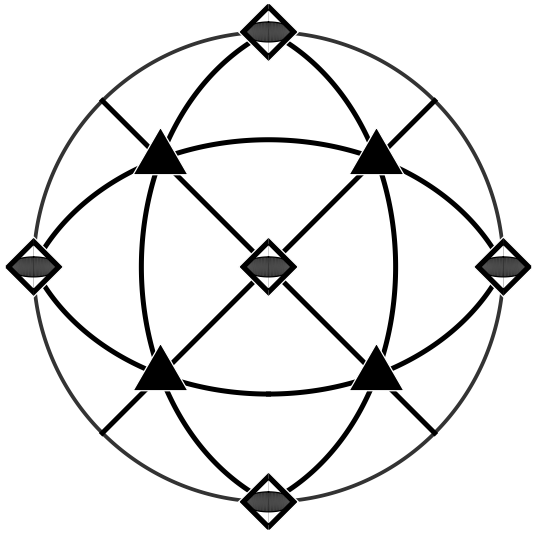
```
CS.Laue
CS.properGroup
CS.properSubGroup
```



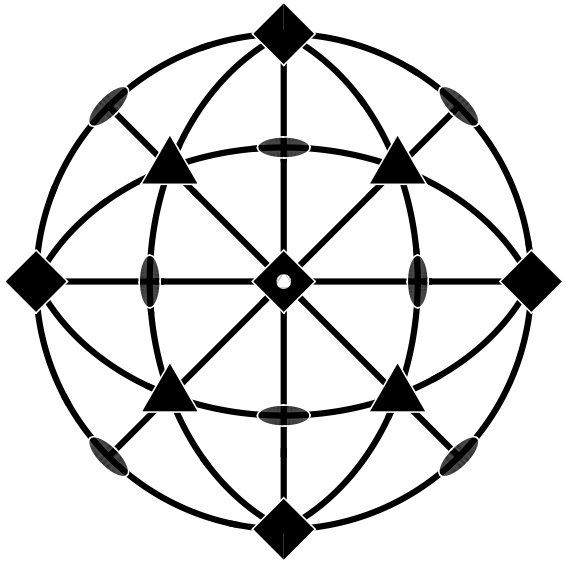




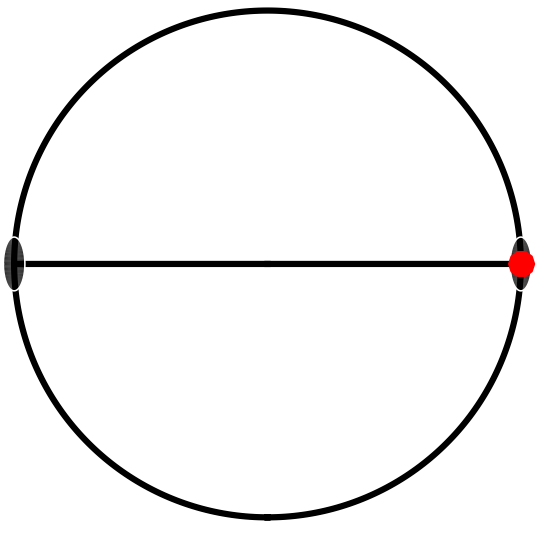
432



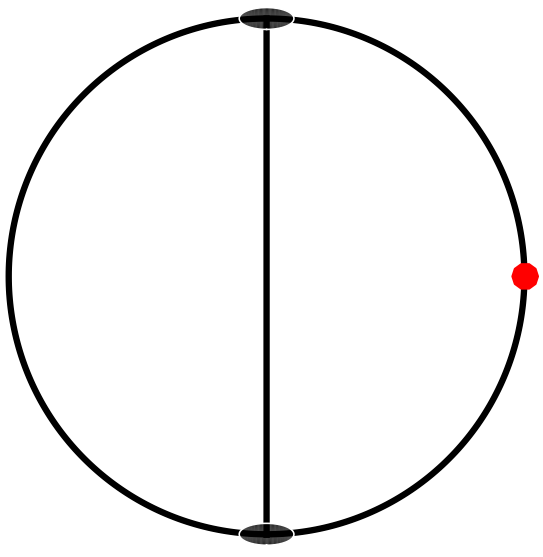
$\bar{4}3m$



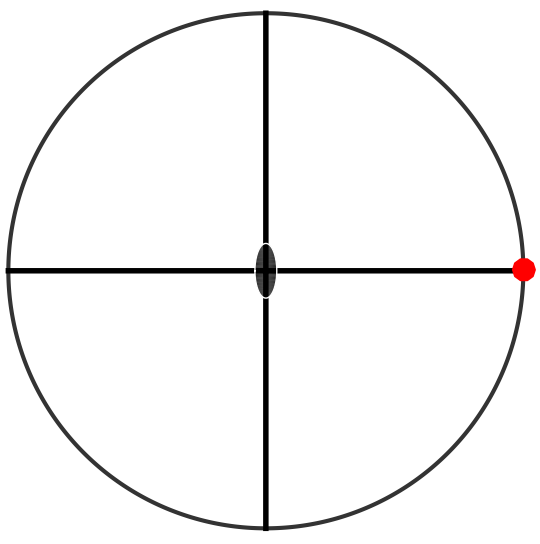
$m\bar{3}m$



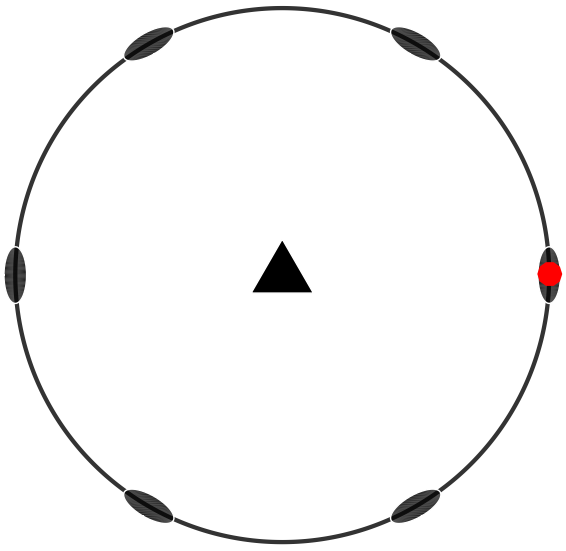
$2mm$



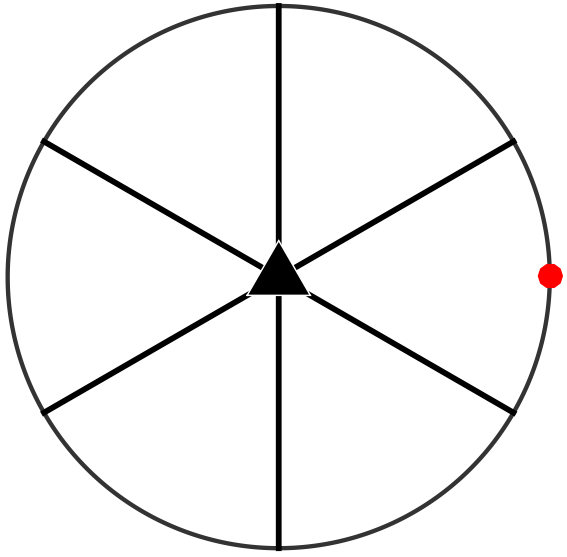
$m2m$



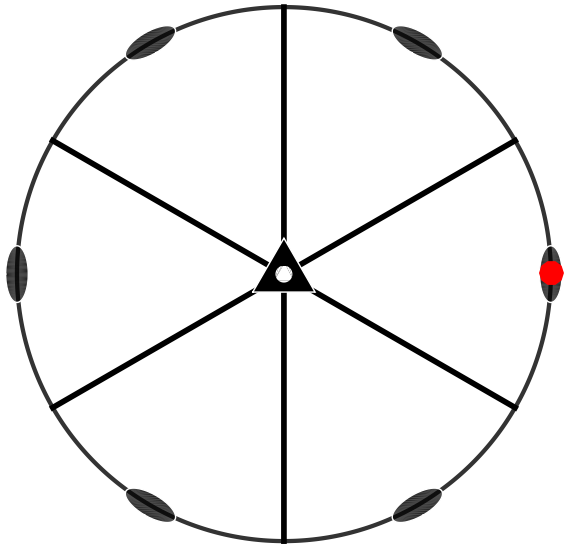
$mm2$



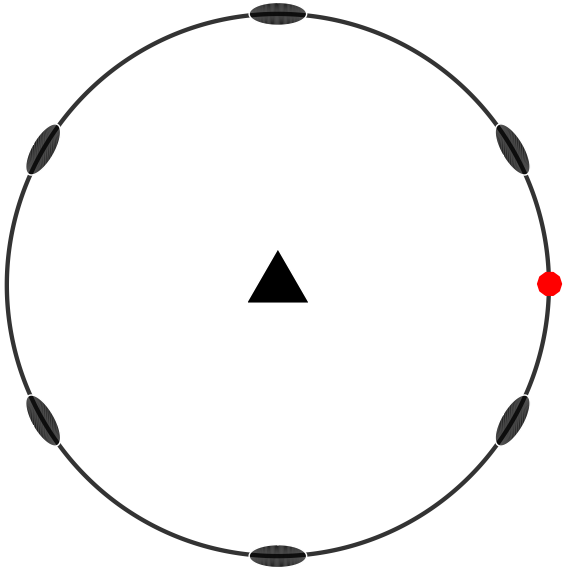
321



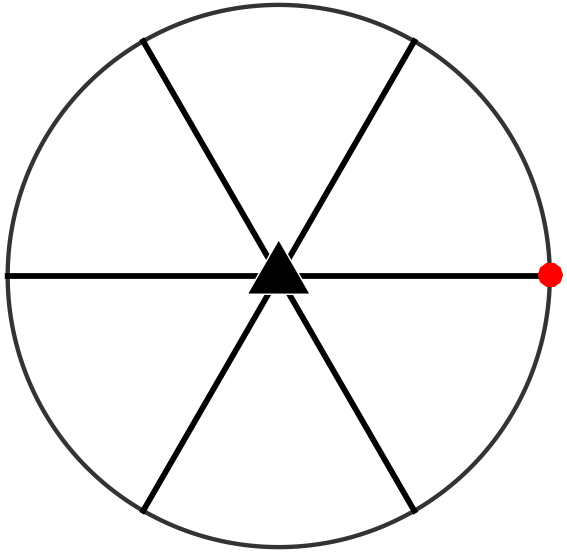
$3m1$



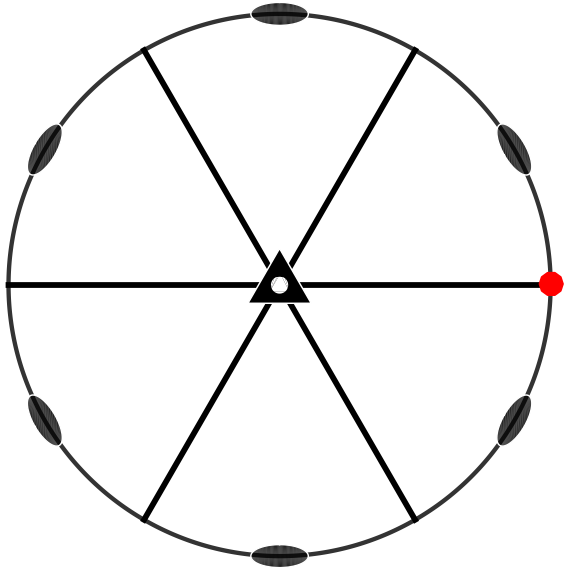
$\bar{3}m1$



312



$31m$



$\bar{3}1m$

Plotting conventions

directions with respect to the sample frame → `vector3d`

EBSD maps, grain maps, pole figures, field tensors, grain properties, grain boundary trace, misorientation axes, slip direction

```
plotx2east, plotx2north, plotx2west, plotx2south
plotzOutOfPlane, plotzIntoPlane
```

directions with respect to the crystal frame → `Miller`

inverse pole figures, misorientation axes, ipf color keys, matter tensors, slip directions,

```
plota2east, plota2north, plota2west, plota2south
plotb2east, plotb2north, plotb2west, plotb2south
```

The above commands do NOT change coordinates.

```
rot = rotation.byAxisAngle(vector3d.Z,90*degree)
ebsd_rot = rotate(ebsd,rot)
```

Plotting conventions

directions with respect to the sample frame → `vector3d`

EBSD maps, grain maps, pole figures, field tensors, grain properties, grain boundary trace, misorientation axes, slip direction

```
plotx2east, plotx2north, plotx2west, plotx2south
plotzOutOfPlane, plotzIntoPlane
```

directions with respect to the crystal frame → `Miller`

inverse pole figures, misorientation axes, ipf color keys, matter tensors, slip directions,

```
plota2east, plota2north, plota2west, plota2south
plotb2east, plotb2north, plotb2west, plotb2south
```

The above commands do NOT change coordinates.

```
rot = rotation.byAxisAngle(vector3d.Z,90*degree)
ebsd_rot = rotate(ebsd,rot)
```

Plotting conventions

directions with respect to the sample frame → `vector3d`

EBSD maps, grain maps, pole figures, field tensors, grain properties, grain boundary trace, misorientation axes, slip direction

```
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plotzOutOfPlane, plotzIntoPlane
```

directions with respect to the crystal frame → `Miller`

inverse pole figures, misorientation axes, ipf color keys, matter tensors, slip directions,

```
plota2east, plota2north, plota2west, plota2south
plotb2east, plotb2north, plotb2west, plotb2south
```

The above commands do NOT change coordinates.

```
rot = rotation.byAxisAngle(vector3d.Z,90*degree)
ebsd_rot = rotate(ebsd,rot)
```

Unit Cell, Reciprocal and Orthogonal Coordinate System

The unit cell of a crystal is specified by the length of its three edges $\vec{a}, \vec{b}, \vec{c}$ and by angles α, β, γ they enclose.

```
C = crystalSymmetry('1',[a b c],[alpha beta gamma])
```

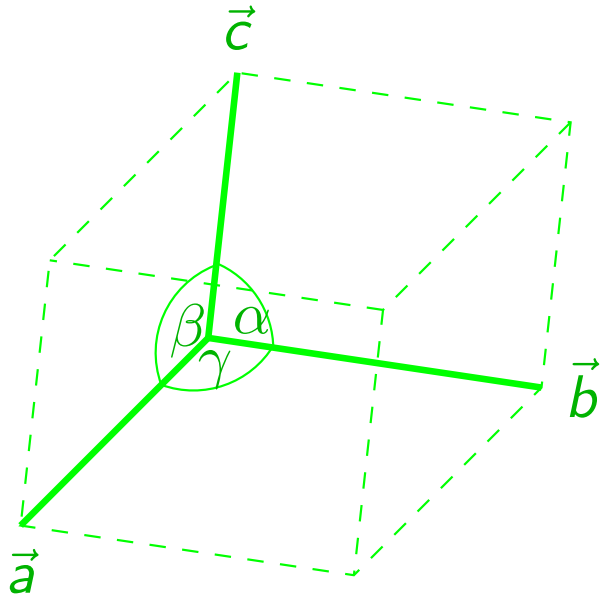
The axes of the reciprocal lattice are defined orthogonal to $\vec{a}, \vec{b}, \vec{c}$, i.e.

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V}, \quad \vec{b}^* = \frac{\vec{c} \times \vec{a}}{V}, \quad \vec{c}^* = \frac{\vec{a} \times \vec{b}}{V}$$

with $V = \vec{a} \cdot (\vec{b} \times \vec{c})$ volume of the unit cell

We will need also an orthogonal coordinate system $(\vec{x}, \vec{y}, \vec{z})$ fixed to the crystal.

There are different conventions.



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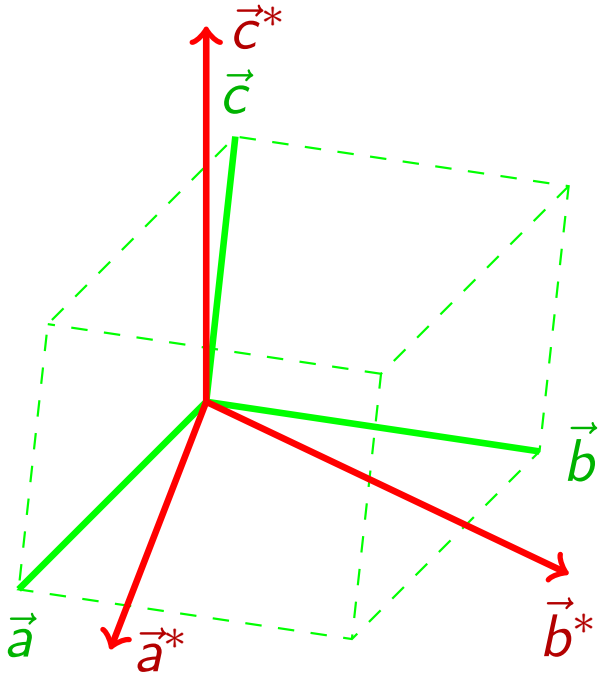

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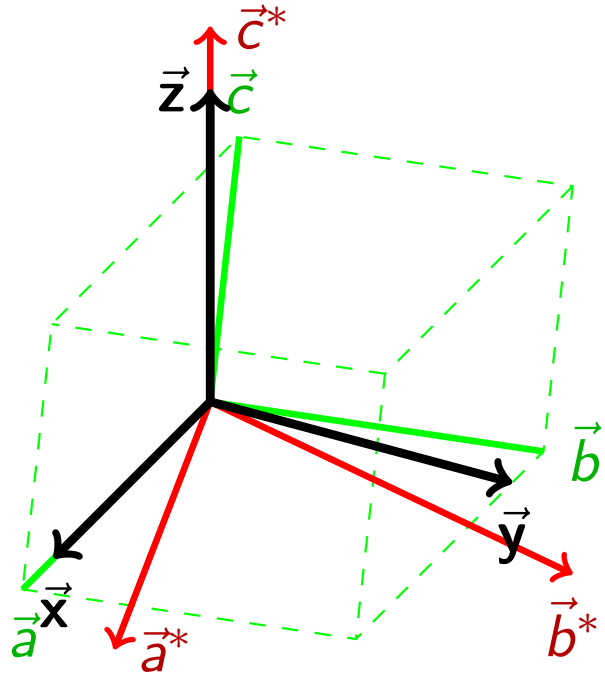


```
CS = crystalSymmetry('321',[a b c],'X||a','Z||c*')
```

Unit Cell, Reciprocal and Orthogonal Coordinate System

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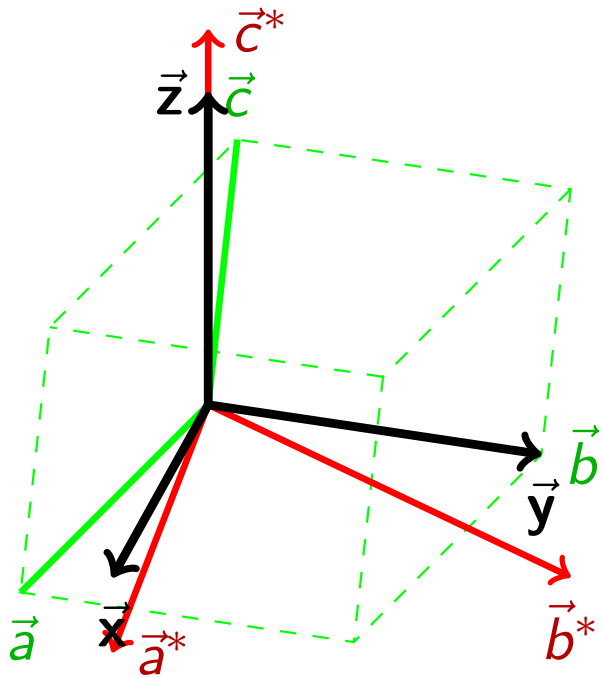


```
CS = crystalSymmetry('321',[a b c],'X||b','Z||c*')
```

The alignment of $\vec{x}$, $\vec{y}$, $\vec{z}$ is important as the Euler angles refer to them.

Unit Cell, Reciprocal and Orthogonal Coordinate System

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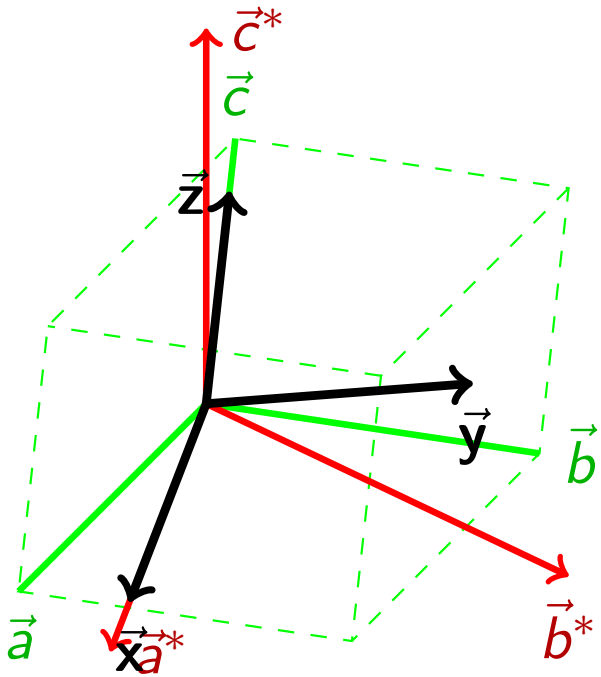



```
CS = crystalSymmetry('321',[a b c],'X||a*','Z||c')
```

The alignment of $\vec{x}$, $\vec{y}$, $\vec{z}$ is important as the Euler angles refer to them.

Miller Indices - Crystal Fixed Directions

A direction with respect to the crystal coordinate system **C**

$$\vec{m} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}.$$

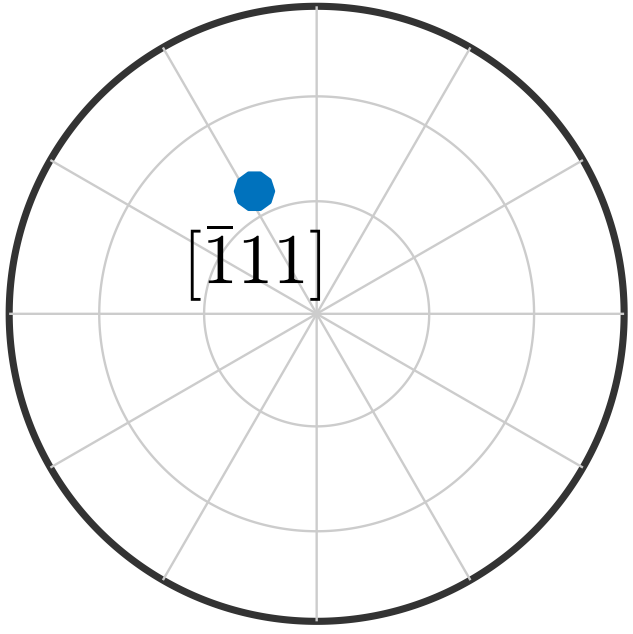
Miller Indices - Crystal Fixed Directions

A direction with respect to the crystal coordinate system **C**

$$\vec{m} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}.$$

```
CS = crystalSymmetry('mmm',[1 2 3])
m  = Miller(-1,1,1,CS,'uvw')
```

```
m = Miller (show methods, plot)
  size: 1 x 1
  symmetry: mmm
  u -1
  v 1
  w 1
```




```
plot(m,'labeled')
```

Miller Indices - Crystal Fixed Directions

A direction with respect to the crystal coordinate system **C**

$$\vec{m} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}.$$

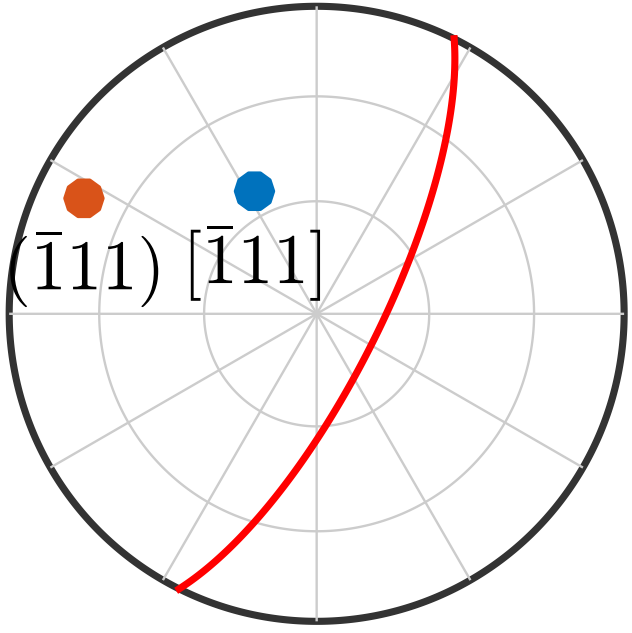
```
CS = crystalSymmetry('mmm',[1 2 3])
m  = Miller(-1,1,1,CS,'uvw')
```

A direction in reciprocal coordinates

$$\vec{n} = h \cdot \vec{a}^* + k \cdot \vec{b}^* + \ell \cdot \vec{c}^*.$$

```
n  = Miller(-1,1,1,CS,'hkl')
```

```
n = Miller (show methods, plot)
  size: 1 x 1
  symmetry: mmm
  h -1
  k 1
  l 1
```




```
plot(m,'labeled')
```

```
hold on
plot(n,'labeled')
```

```
plot(n,'plane')
```

Miller Indices - Crystal Fixed Directions

A direction with respect to the crystal coordinate system **C**

$$\vec{m} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}.$$

```
CS = crystalSymmetry('mmm',[1 2 3])
m  = Miller(-1,1,1,CS,'uvw')
```

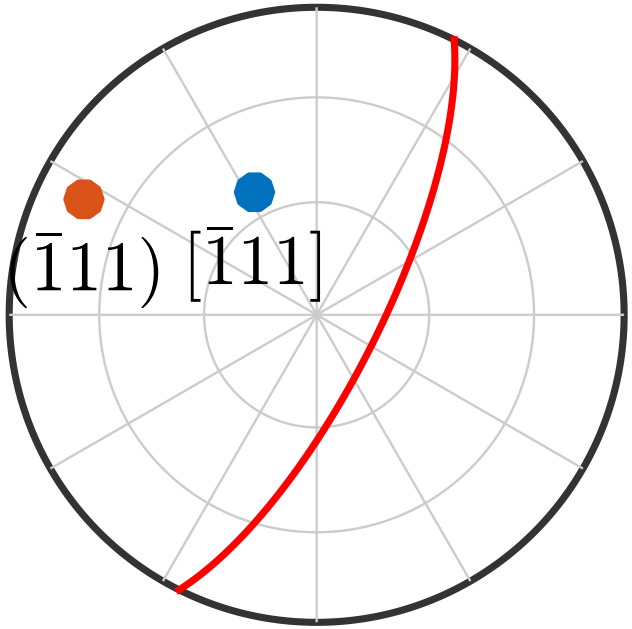
A direction in reciprocal coordinates

$$\vec{n} = h \cdot \vec{a}^* + k \cdot \vec{b}^* + \ell \cdot \vec{c}^*.$$

```
n  = Miller(-1,1,1,CS,'hkl')
```

A direction in the orthogonal coordinate system

```
m = Miller(vector3d.X,CS)
m = Miller.byPolar(theta,rho,CS)
```

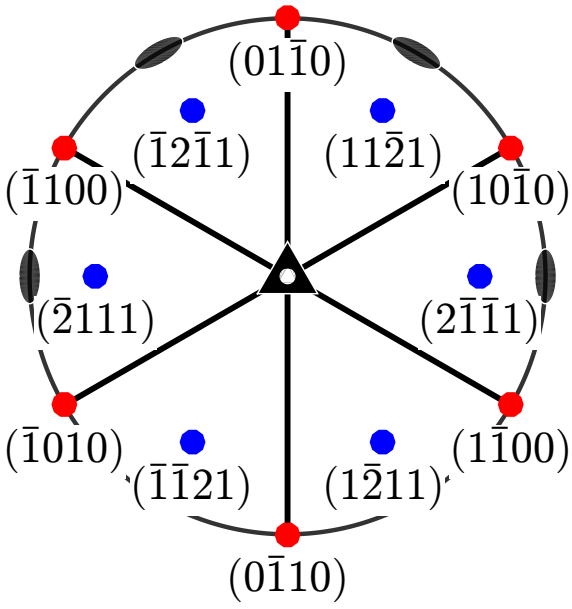


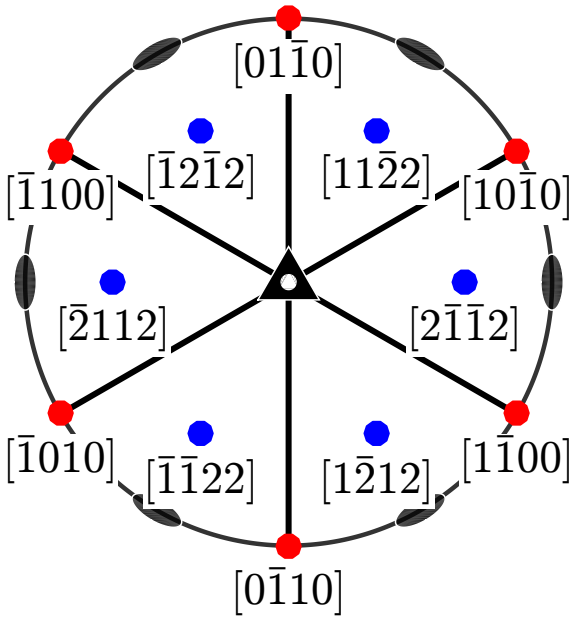

```
plot(m,'labeled')
```

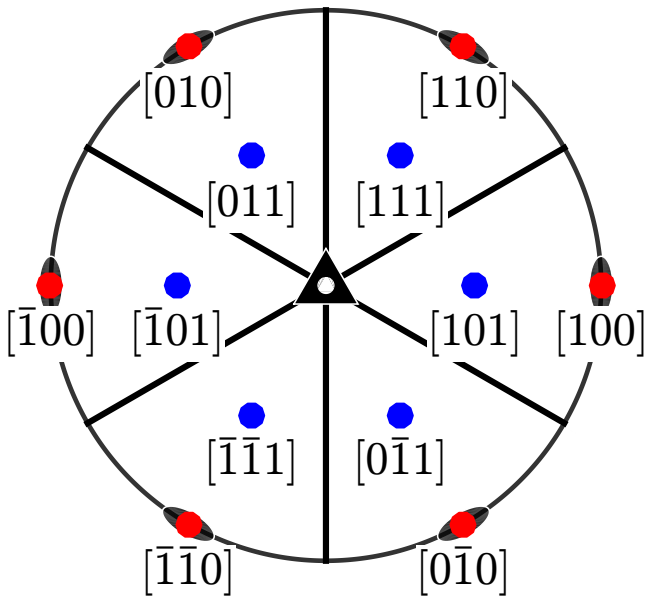
```
hold on
plot(n,'labeled')
```

```
plot(n,'plane')
```

Trigonal and Hexagonal Symmetries







lists of crystal directions

```
m = Miller({1 0 -1 0},{1 1 -2 1},CS,'hkil')
m = Miller({1 0 -1 0},{1 1 -2 2},CS,'UVTW')
m = Miller({1 0 0},{1 0 1},CS,'uvw')
```

plot all symmetrically equivalent directions

```
plot(m,'symmetrised','labeled')
```

Calculating with Crystal Directions

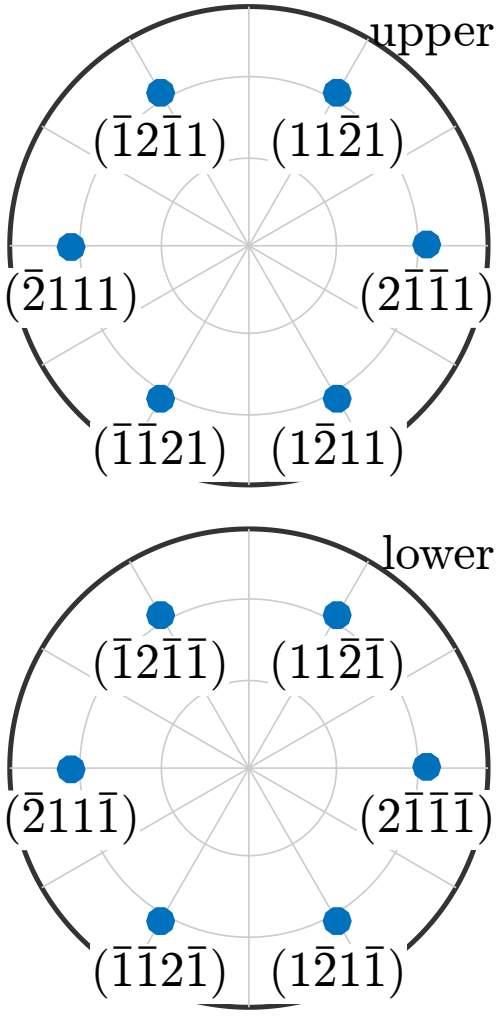
Find all symmetrically equivalent directions

```
CS = crystalSymmetry.load('quartz')
n1 = Miller({2 -1 -1 1},CS,'hkil')
symmetrise(n1)
```

```
ans = Miller (show methods, plot)
  size: 6 x 1
  mineral: Quartz (321, X||a*, Y||b, Z||c*)
   h  2  2 -1 -1 -1 -1
   k -1 -1  2 -1 -1  2
   i -1 -1 -1  2  2 -1
   l  1 -1  1 -1  1 -1
```

angle modulo symmetry

equivalent directions are treated as equal



Calculating with Crystal Directions

Find all symmetrically equivalent directions

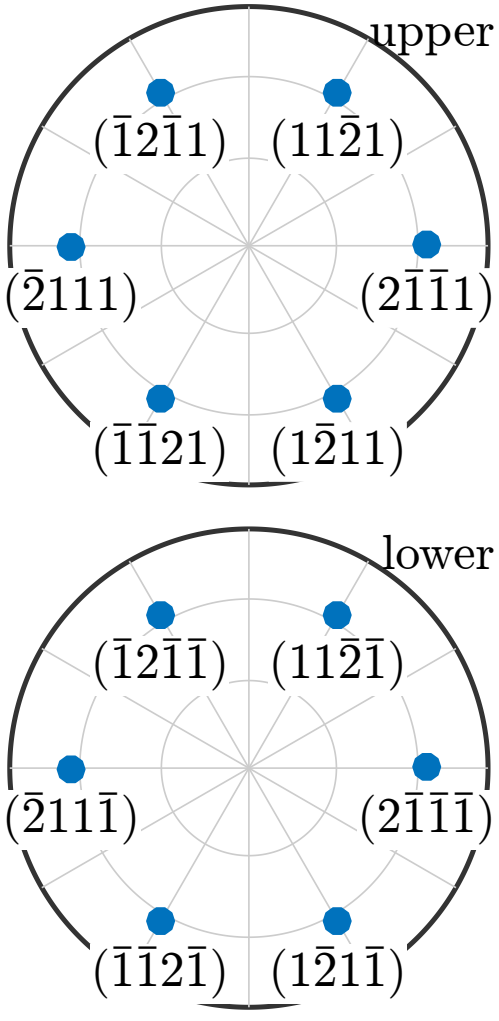
```
CS = crystalSymmetry.load('quartz')
n1 = Miller({2 -1 -1 1},CS,'hkil')
symmetrise(n1)
```

angle modulo symmetry

```
n2 = Miller({-2 1 1 -2},CS,'hkil')
angle(n1,n2) / degree
```

```
ans =
   52.0312
```

equivalent directions are treated as equal



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Find all symmetrically equivalent directions

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CS = crystalSymmetry.load('quartz')
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symmetrise(n1)
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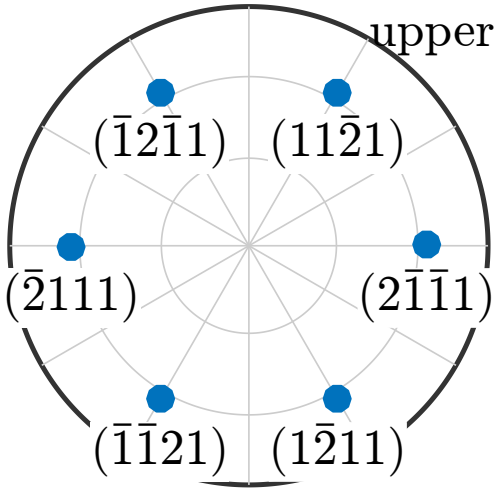
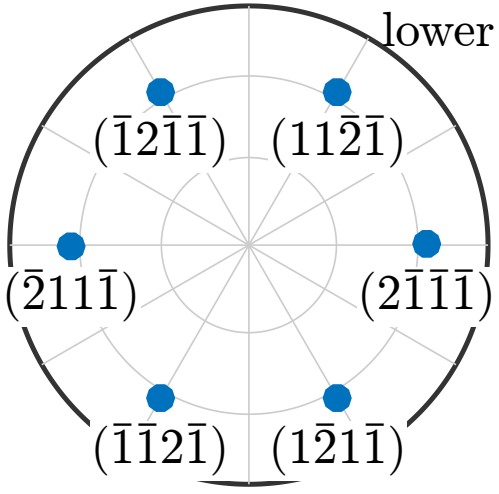


angle modulo symmetry

```
n2 = Miller({-2 1 1 -2},CS,'hkil')
angle(n1,n2,'noSymmetry') / degree
```

```
ans =
  162.1674
```

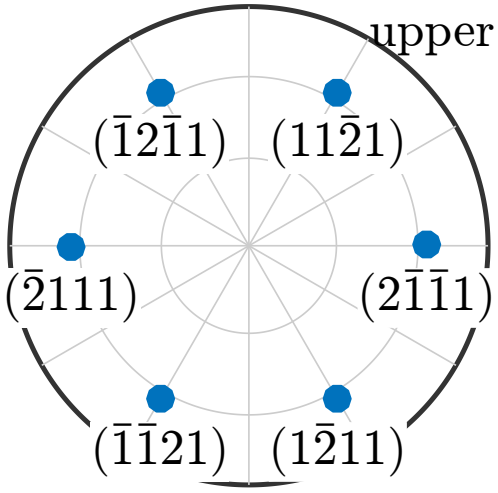


equivalent directions are treated as equal

Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = crystalSymmetry.load('quartz')
n1 = Miller({2 -1 -1 1},CS,'hkil')
symmetrise(n1)
```



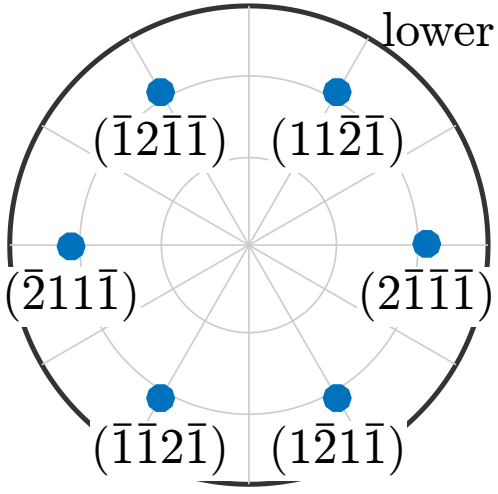
angle modulo symmetry

```
n2 = Miller({-2 1 1 -2},CS,'hkil')
angle(n1,n2,'noSymmetry') / degree
```

equivalent directions are treated as equal

```
unique(n1.symmetrise)
```

```
ans = Miller (show methods, plot)
 size: 1 x 1
 mineral: Quartz (321, X||a*, Y||b, Z||c*)
  h  2
  k -1
  i -1
  l  1
```



Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = crystalSymmetry.load('quartz')
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```
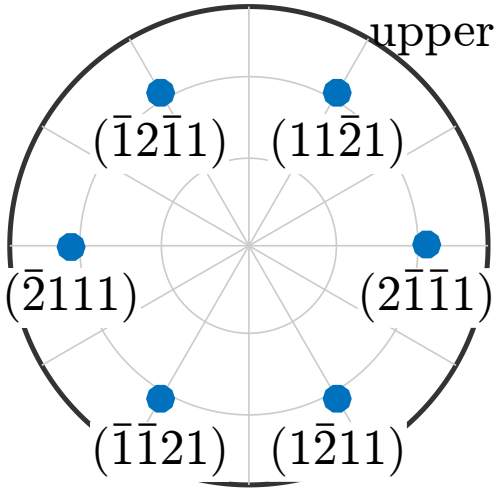
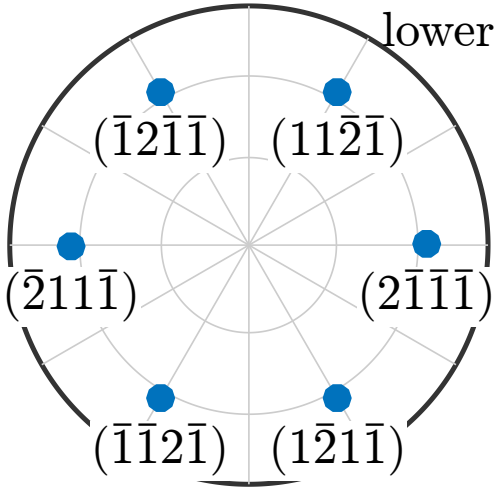



angle modulo symmetry

```
n2 = Miller({-2 1 1 -2},CS,'hkil')
angle(n1,n2,'noSymmetry') / degree
```

equivalent directions are treated as equal

```
unique(n1.symmetrise,'noSymmetry')
```



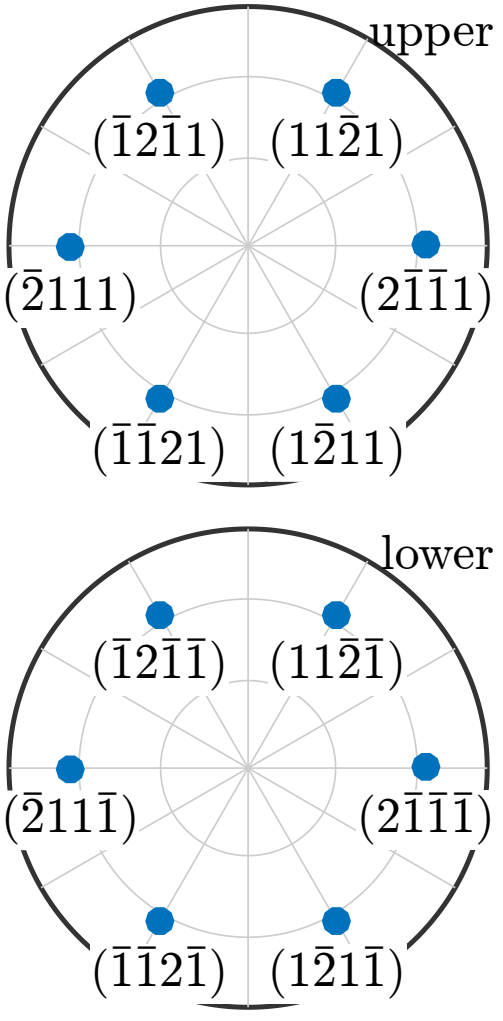

```
ans = Miller (show methods, plot)
 size: 6 x 1
 mineral: Quartz (321, X||a*, Y||b, Z||c*)
  h -1 -1 -1 -1  2  2
  k -1 -1  2  2 -1 -1
  i  2  2 -1 -1 -1 -1
  l  1 -1 -1  1  1 -1
```

Calculating with Crystal Directions

Find the zone axis of two lattice planes

```
CS = crystalSymmetry.load('quartz')
n1 = Miller({1 -1 0 0},CS,'hkil')
n2 = Miller({0 1 -1 0},CS,'hkil')
zoneAxis = cross(n1,n2)
```

```
zoneAxis = Miller (show methods, plot)
  size: 1 x 1
  mineral: Quartz (322, X||a*, Y||b, Z||c*)
   U       0
   V       0
   T       0
   W -0.0265
```



Find the plane spanned by two directions

best normal to a list of directions

```
d = Miller({2 -1 -1 1},cs,'UVTW')
n = perp(d.symmetrise)
```

Calculating with Crystal Directions

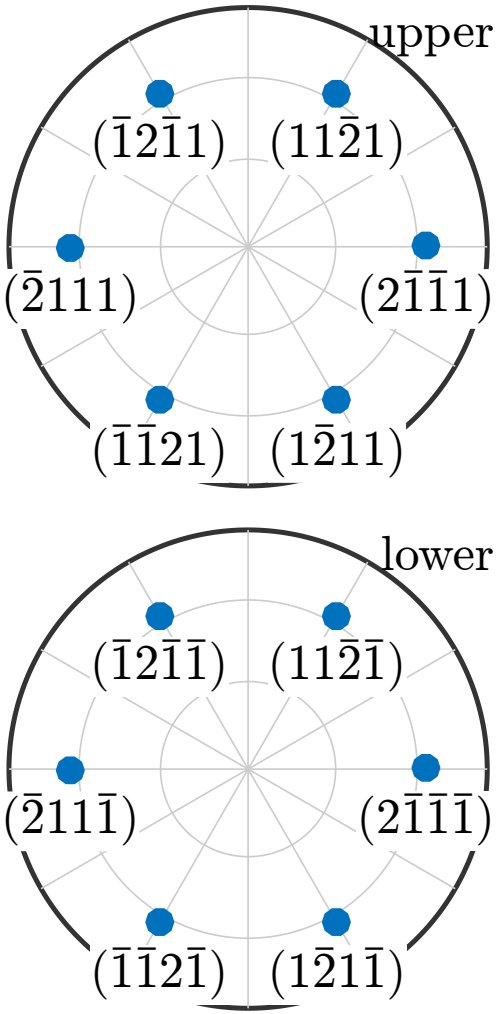
Find the zone axis of two lattice planes

```
CS = crystalSymmetry.load('quartz')
n1 = Miller({1 -1 0 0},CS,'hkil')
n2 = Miller({0 1 -1 0},CS,'hkil')
zoneAxis = cross(n1,n2)
```

Find the plane spanned by two directions

```
d1 = Miller({1 -1 0 0},CS,'UVTW')
d2 = Miller({1 -1 0 1},CS,'UVTW')
 n = cross(d1,d2)
```

```
n = Miller (show methods, plot)
  size: 1 x 1
  mineral: Quartz (321, X||a*, Y||b, Z||c*)
   h -12.5701
   k -12.5701
   i  25.1403
   l         0
```



best normal to a list of directions

Calculating with Crystal Directions

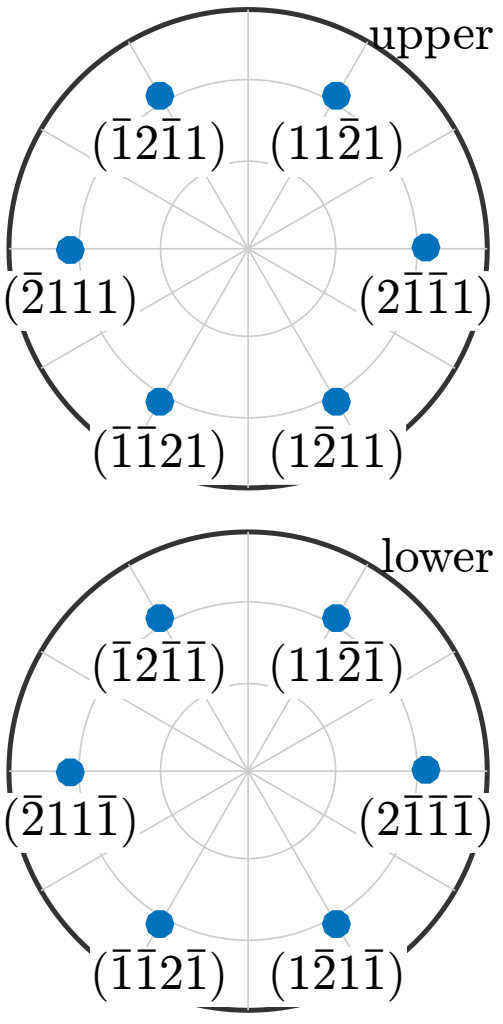
Find the zone axis of two lattice planes

```
CS = crystalSymmetry.load('quartz')
n1 = Miller({1 -1 0 0},CS,'hkil')
n2 = Miller({0 1 -1 0},CS,'hkil')
zoneAxis = cross(n1,n2)
```

Find the plane spanned by two directions

```
d1 = Miller({1 -1 0 0},CS,'UVTW')
d2 = Miller({1 -1 0 1},CS,'UVTW')
 n = round(cross(d1,d2))
```

```
n = Miller (show methods, plot)
  size: 1 x 1
  mineral: Quartz (321, X||a*, Y||b, Z||c*)
   h -1
   k -1
   i  2
   l  0
```



round is not **normalize**!

Calculating with Crystal Directions

Find the zone axis of two lattice planes

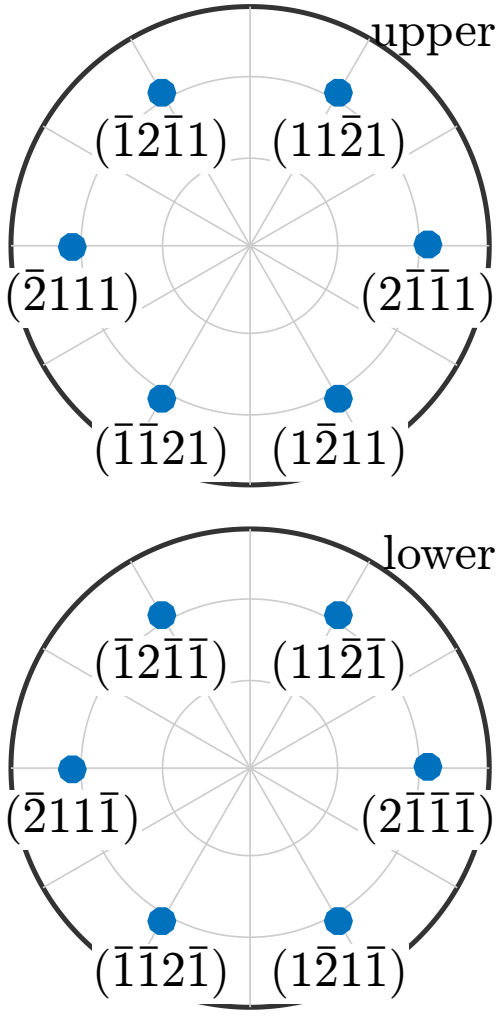
```
CS = crystalSymmetry.load('quartz')
n1 = Miller({1 -1 0 0},CS,'hkil')
n2 = Miller({0 1 -1 0},CS,'hkil')
zoneAxis = cross(n1,n2)
```

Find the plane spanned by two directions

```
d1 = Miller({1 -1 0 0},CS,'UVTW')
d2 = Miller({1 -1 0 1},CS,'UVTW')
 n = round(cross(d1,d2))
```

best normal to a list of directions

```
d = Miller({2 -1 -1 1},cs,'UVTW')
n = perp(d.symmetrise)
```



Crystal Orientations

Let a vector $\vec{v}$ be given by specimen coordinates $(r_1, r_2, r_3)^t$ and crystal coordinates $(h_1, h_2, h_3)^t$, i.e.,

$$\vec{v} = r_1\vec{X} + r_2\vec{Y} + r_3\vec{Y} = h_1\vec{x} + h_2\vec{y} + h_3\vec{z}.$$

The coordinate transform $\mathbf{O}$ with

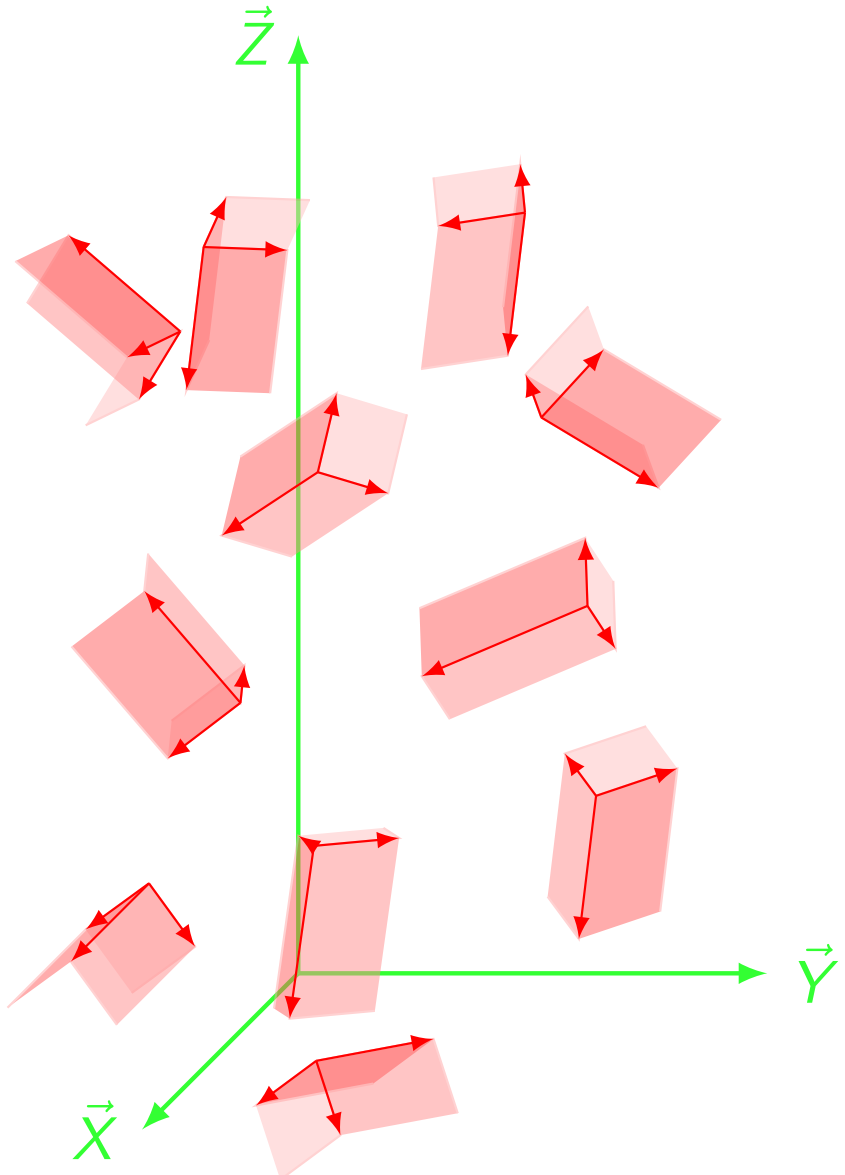
$$(r_1, r_2, r_3)^t = \mathbf{O}\,(h_1, h_2, h_3)^t$$

is called crystal orientation.

Bunge specimen $\rightarrow$ crystal

MTEX crystal $\rightarrow$ specimen

an orientation $\mathbf{O}$ is well defined only modulo crystal symmetry.



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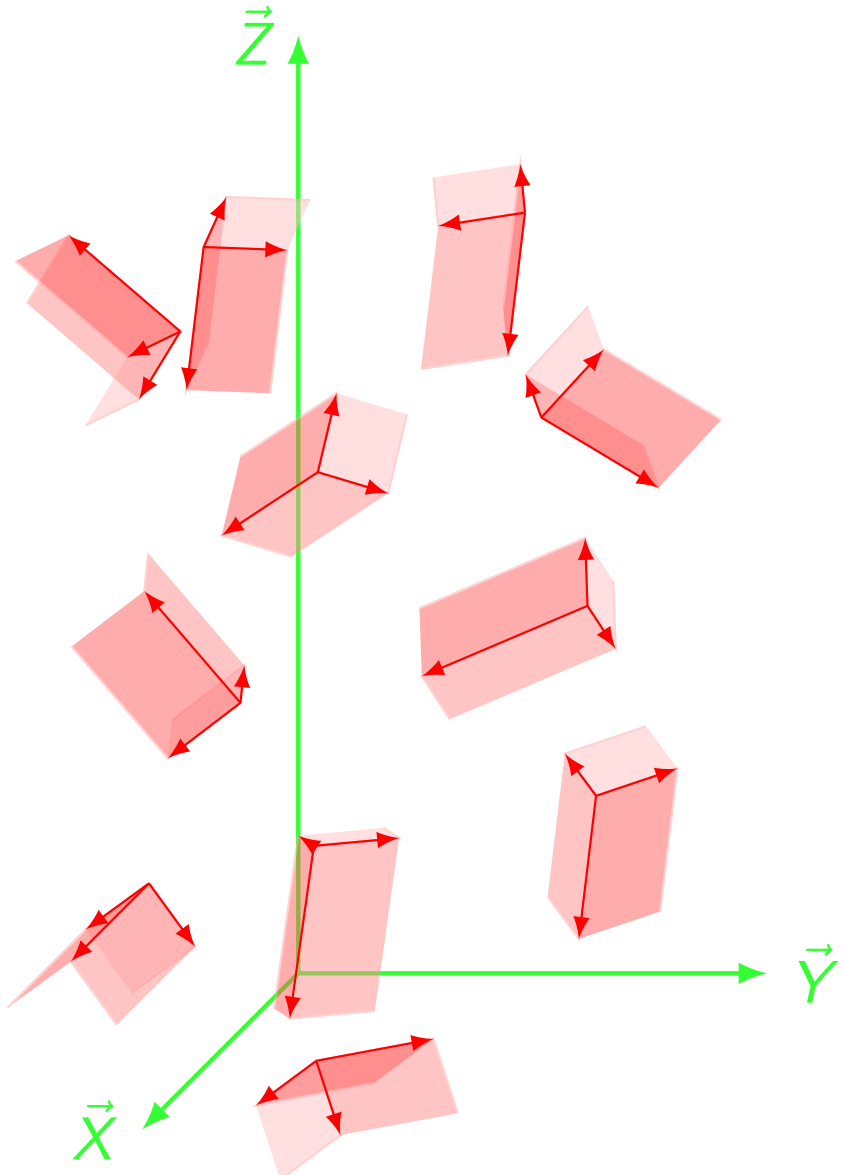

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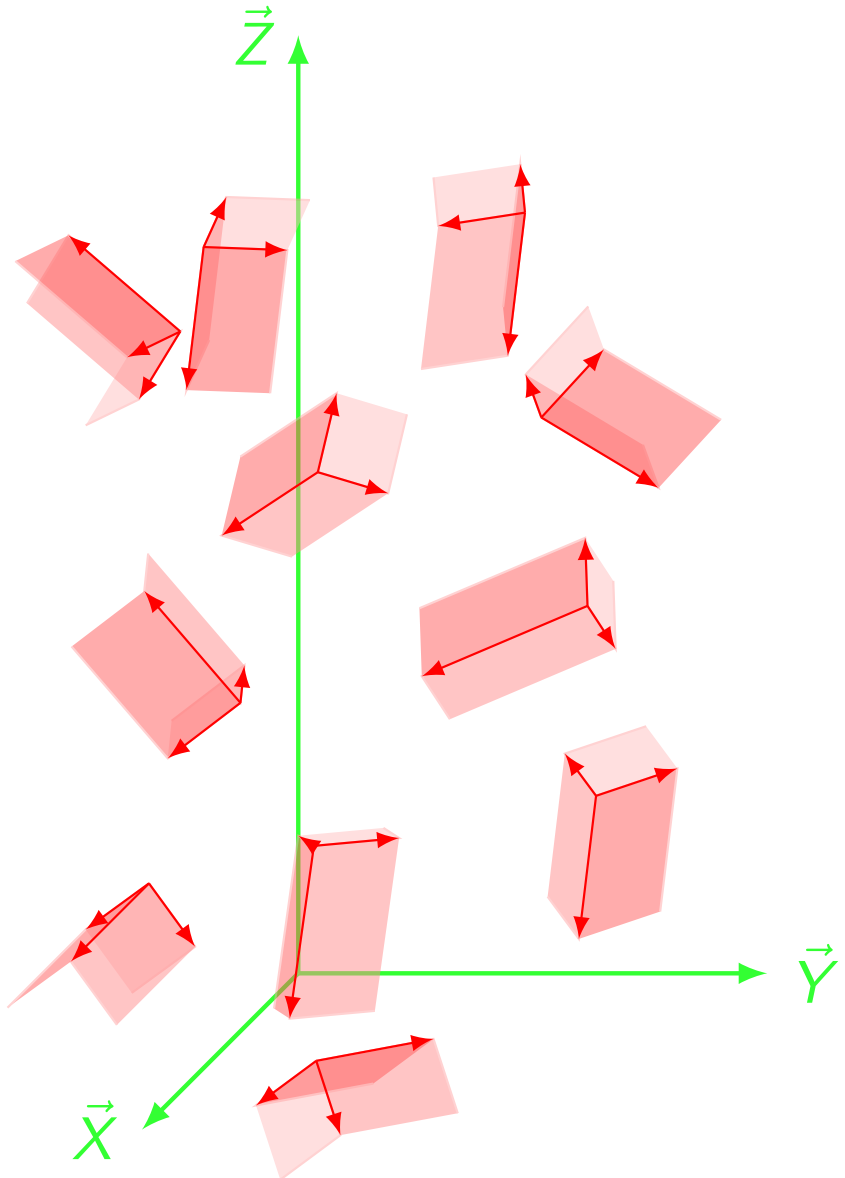

Crystal Orientations

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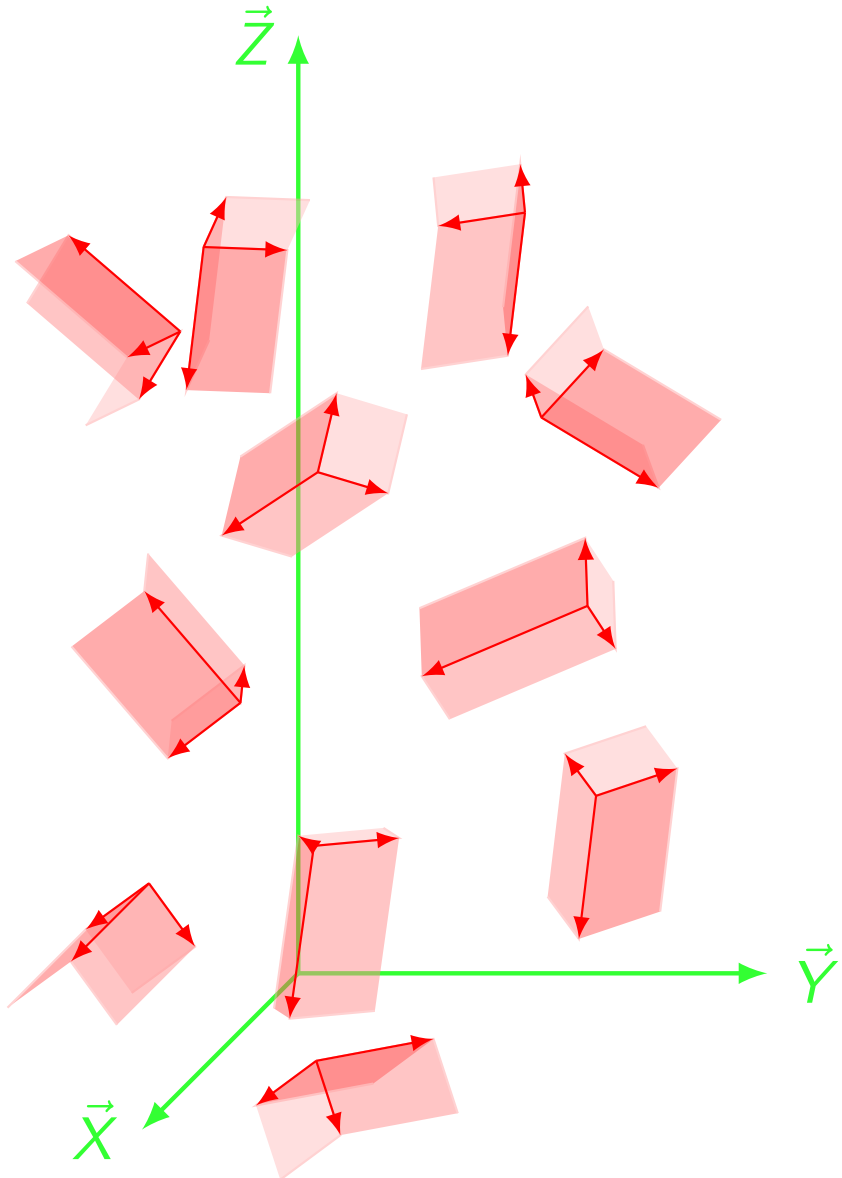

Defining Orientations

define orientations by Euler angles

```
CS = crystalSymmetry('321')
SS = specimenSymmetry('1') % optional
O  = orientation.byEuler(10*degree,5*degree,0,CS,SS)
```

```
O = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry: 321, X||a*, Y||b, Z||c*
  sample symmetry : 1

  Bunge Euler angles in degree
  phi1   Phi   phi2   Inv.
    10     5      0     0
```

import orientations

```
O = orientation.load('filename',CS,SS,...
    'ColumnNames',{'phi1','Phi','phi2'})
```

define orientations by Miller indices

```
O = orientation.byMiller([h k l],[u v w],CS,SS)
```

Defining Orientations

define orientations by Euler angles

```
CS = crystalSymmetry('321')
SS = specimenSymmetry('1') % optional
O  = orientation.byEuler(10*degree,5*degree,0,CS,SS)
```

import orientations

```
O  = orientation.load('filename',CS,SS,...
     'ColumnNames',{'phi1','Phi','phi2'})
```

```
O = orientation (show methods, plot)
  size: 1000 x 1
  crystal symmetry: 321, X||a*, Y||b, Z||c*
  sample symmetry : 1
```

define orientations by Miller indices

```
O  = orientation.byMiller([h k l],[u,v,w],CS,SS)
```

standard orientations: Cube, CubeND22, CubeND45, CubeRD, Goss, invGoss, Copper, Copper2, SR, SR2, SR3, SR4, Brass, Brass2,

Defining Orientations

define orientations by Euler angles

```
CS = crystalSymmetry('321')
SS = specimenSymmetry('1') % optional
O  = orientation.byEuler(10*degree,5*degree,0,CS,SS)
```

import orientations

```
O  = orientation.load('filename',CS,SS,...
     'ColumnNames',{'phi1','Phi','phi2'})
```

define orientations by Miller indices

```
O  = orientation.byMiller([h k l],[u,v,w],CS,SS)
```

standard orientations: Cube, CubeND22, CubeND45, CubeRD, Goss, invGoss, Copper, Copper2, SR, SR2, SR3, SR4, Brass, Brass2, PLage, PLage2, QLage, QLage2, QLage3, QLage4

```
O  = orientation.brass(CS,SS)
```

Defining Orientations

define orientations by Euler angles

```
CS = crystalSymmetry('321')
SS = specimenSymmetry('1') % optional
O  = orientation.byEuler(10*degree,5*degree,0,CS,SS)
```

import orientations

```
O  = orientation.load('filename',CS,SS,...
     'ColumnNames',{'phi1','Phi','phi2'})
```

define orientations by Miller indices

```
O  = orientation.byMiller([h k l],[u,v,w],CS,SS)
```

standard orientations: `Cube`, `CubeND22`, `CubeND45`, `CubeRD`, `Goss`, `invGoss`, `Copper`, `Copper2`, `SR`, `SR2`, `SR3`, `SR4`, `Brass`, `Brass2`, `PLage`, `PLage2`, `QLage`, `QLage2`, `QLage3`, `QLage4`

```
O  = orientation.brass(CS,SS)
```

Calculating with Orientations

find all symmetrically equivalent orientations

symmetrise(O)

```
ans = orientation (show methods, plot)
  size: 6 x 1
  crystal symmetry: 321, X||a*, Y||b, Z||c*
  sample symmetry : 1

  Roe Euler angles in degree
  Psi  Theta    Phi  Inv.
   10      5      0    0
   10      5    120    0
   10      5    240    0
  190    175     60    0
  190    175    180    0
  190    175    300    0
```

convert crystal into specimen coordinates

```
h = Miller({1 0 -1 0},CS);
r = O * h
```

Calculating with Orientations

find all symmetrically equivalent orientations

```
symmetrise(O)
```

convert crystal into specimen coordinates

```
h = Miller({1 0 -1 0},CS);
r = O * h
```

```
r = vector3d (show methods, plot)
  size: 1 x 1
          x          y          z
  0.984808 0.173648          0
```

convert specimen into crystal coordinates

```
inv(O) * r
```

change specimen coordinates

```
R  = rotation.byAxisAngle(vector3d.Z,90*degree)
O2 = R * O1
```

Calculating with Orientations

find all symmetrically equivalent orientations

```
symmetrise(O)
```

convert crystal into specimen coordinates

```
h = Miller({1 0 -1 0},CS);
r = O * h
```

convert specimen into crystal coordinates

```
inv(O) * r
```

```
ans = Miller (show methods, plot)
  size: 1 x 1
  symmetry: 321, X||a*, Y||b, Z||c*
  h  1
  k  0
  i -1
  l  0
```

change specimen coordinates

Calculating with Orientations

find all symmetrically equivalent orientations

```
symmetrise(O)
```

convert crystal into specimen coordinates

```
h = Miller({1 0 -1 0},CS);
r = O * h
```

convert specimen into crystal coordinates

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inv(O) * r
```

change specimen coordinates

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R  = rotation.byAxisAngle(vector3d.Z,90*degree)
O2 = R * O1
```

Order of multiplication inverse to Bunge convention

Calculating with Orientations

find all symmetrically equivalent orientations

```
symmetrise(O)
```

convert crystal into specimen coordinates

```
h = Miller({1 0 -1 0},CS);
r = O * h
```

convert specimen into crystal coordinates

```
inv(O) * r
```

change specimen coordinates

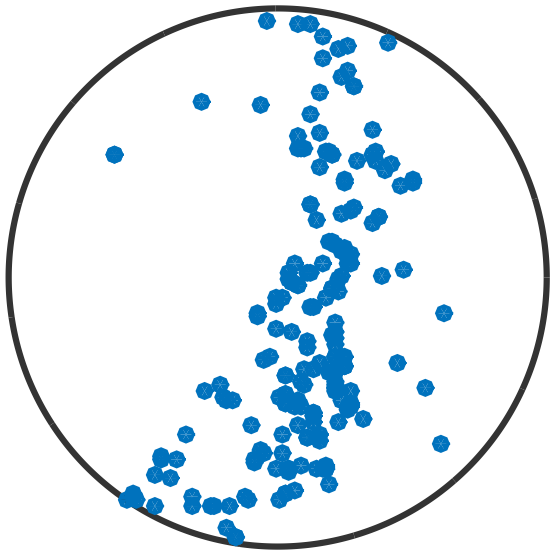
```
R  = rotation.byAxisAngle(vector3d.Z,90*degree)
O2 = R * O1
```

Order of multiplication inverse to Bunge convention

Pole Figures and Inverse Pole Figures

translate lattice planes into specimen coordinates

```
h = Miller({1 0 0}, {0 1 0}, O.CS)
plot(symmetrise(O) * h(1))
plot(O * symmetrise(h(1)))
```



pole figures

translate directions into crystal coordinates

```
r = vector3d.X
plot(symmetrise(inv(O)) * r)
plot(symmetrise(inv(O) * r))
```

inverse pole figures

Pole Figures and Inverse Pole Figures

translate lattice planes into specimen coordinates

```
h = Miller({1 0 0}, {0 1 0}, O.CS)
plot(symmetrise(O) * h(1))
plot(O * symmetrise(h(1)))
```

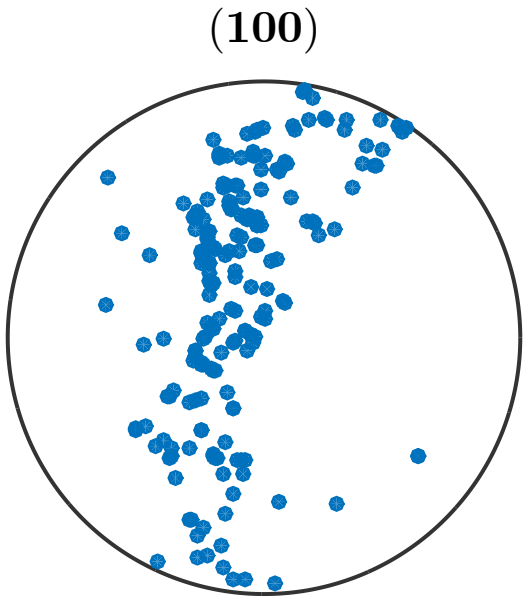
pole figures

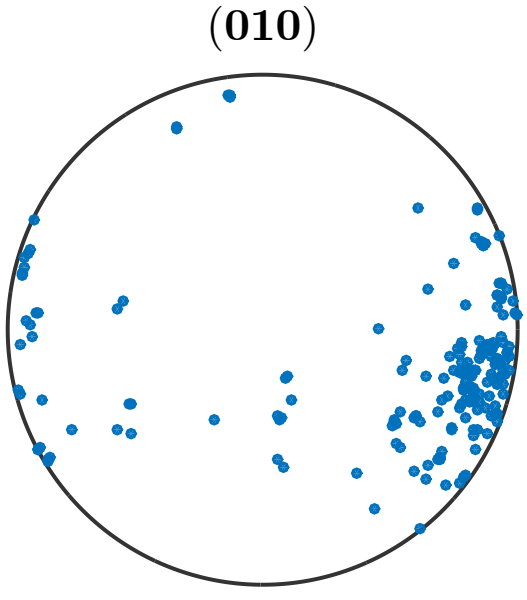
```
plotPDF(O, h)
```

translate directions into crystal coordinates

```
r = vector3d.X
plot(symmetrise(inv(O)) * r)
plot(symmetrise(inv(O) * r))
```

inverse pole figures





Pole Figures and Inverse Pole Figures

translate lattice planes into specimen coordinates

```
h = Miller({1 0 0}, {0 1 0}, O.CS)
plot(symmetrise(O) * h(1))
plot(O * symmetrise(h(1)))
```

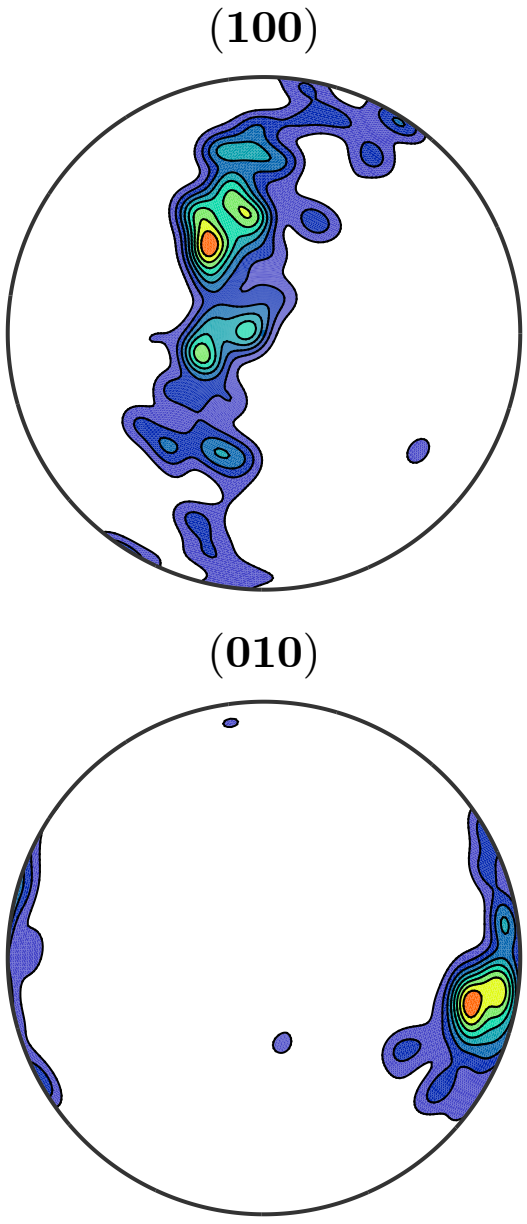
pole figures

```
plotPDF(O,h,'contourf')
```

translate directions into crystal coordinates

```
r = vector3d.X
plot(symmetrise(inv(O)) * r)
plot(symmetrise(inv(O) * r))
```

inverse pole figures



Pole Figures and Inverse Pole Figures

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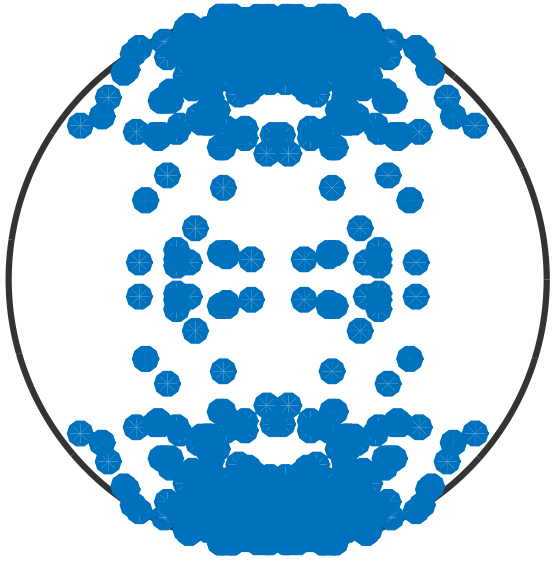
```

inverse pole figures



Pole Figures and Inverse Pole Figures

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h = Miller({1 0 0}, {0 1 0}, O.CS)
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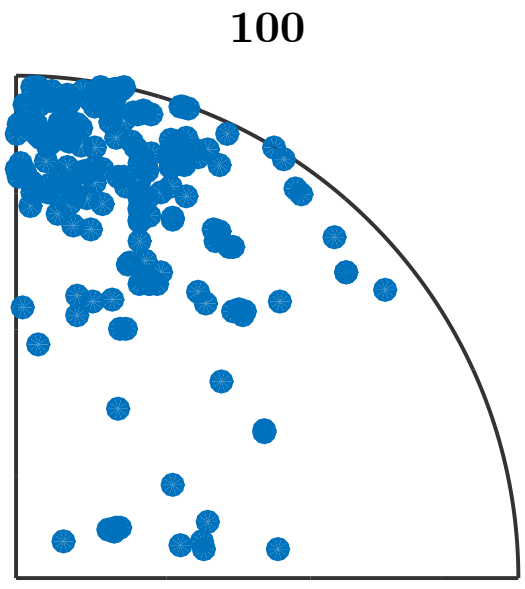
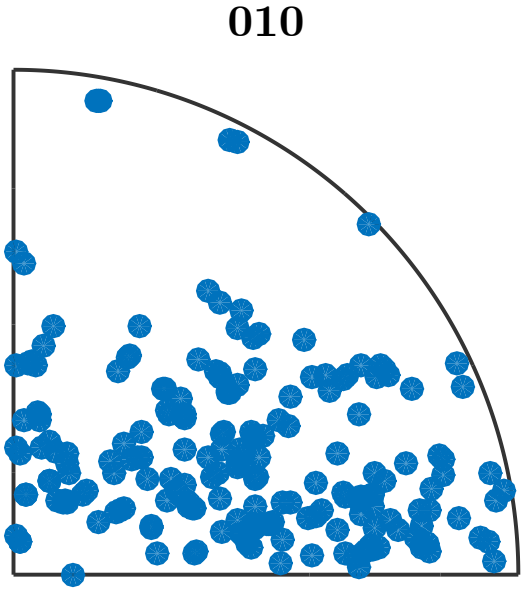


pole figures

```
plotPDF(O,h,'contourf')
```

translate directions into crystal coordinates

```
r = vector3d.X
plot(symmetrise(inv(O)) * r)
plot(symmetrise(inv(O) * r))
```



inverse pole figures

```
v = [vector3d.X, vector3d.Y]
plotIPDF(O,v)
```

Pole Figures and Inverse Pole Figures

translate lattice planes into specimen coordinates

```
h = Miller({1 0 0}, {0 1 0}, O.CS)
plot(symmetrise(O) * h(1))
plot(O * symmetrise(h(1)))
```

pole figures

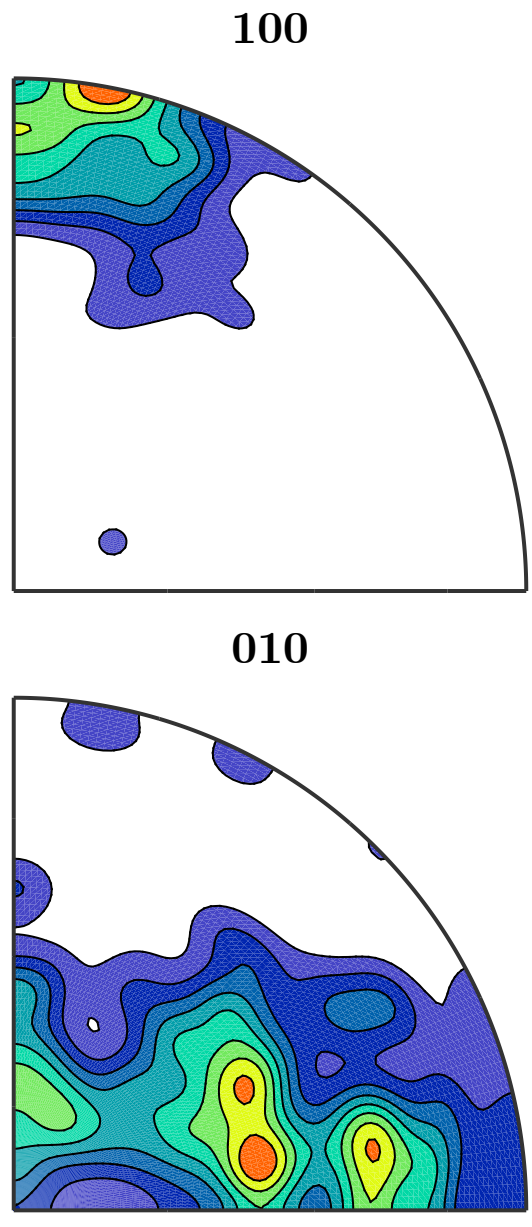
```
plotPDF(O,h,'contourf')
```

translate directions into crystal coordinates

```
r = vector3d.X
plot(symmetrise(inv(O)) * r)
plot(symmetrise(inv(O) * r))
```

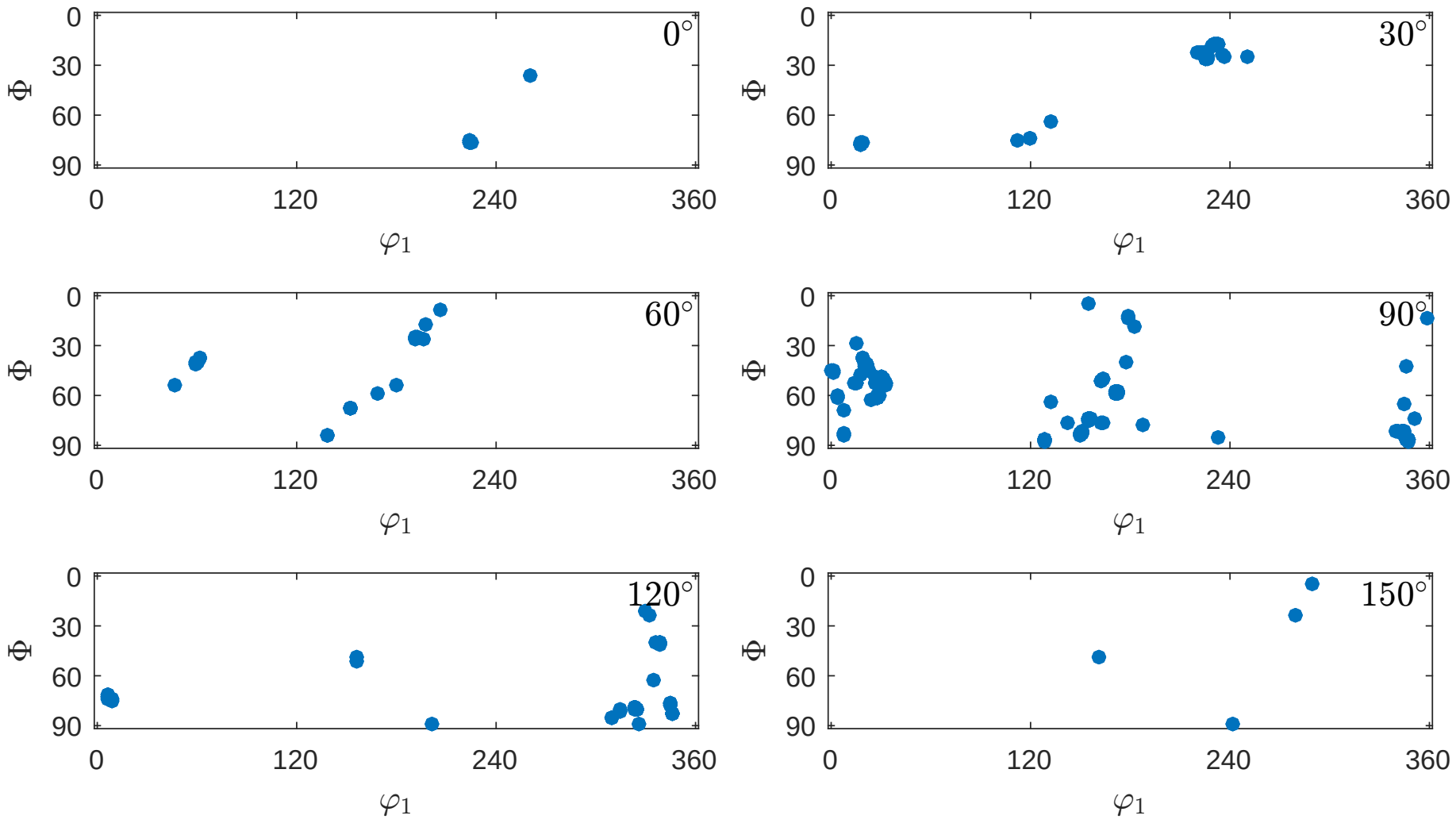
inverse pole figures

```
v = [vector3d.X, vector3d.Y]
plotIPDF(O,v,'contourf')
```



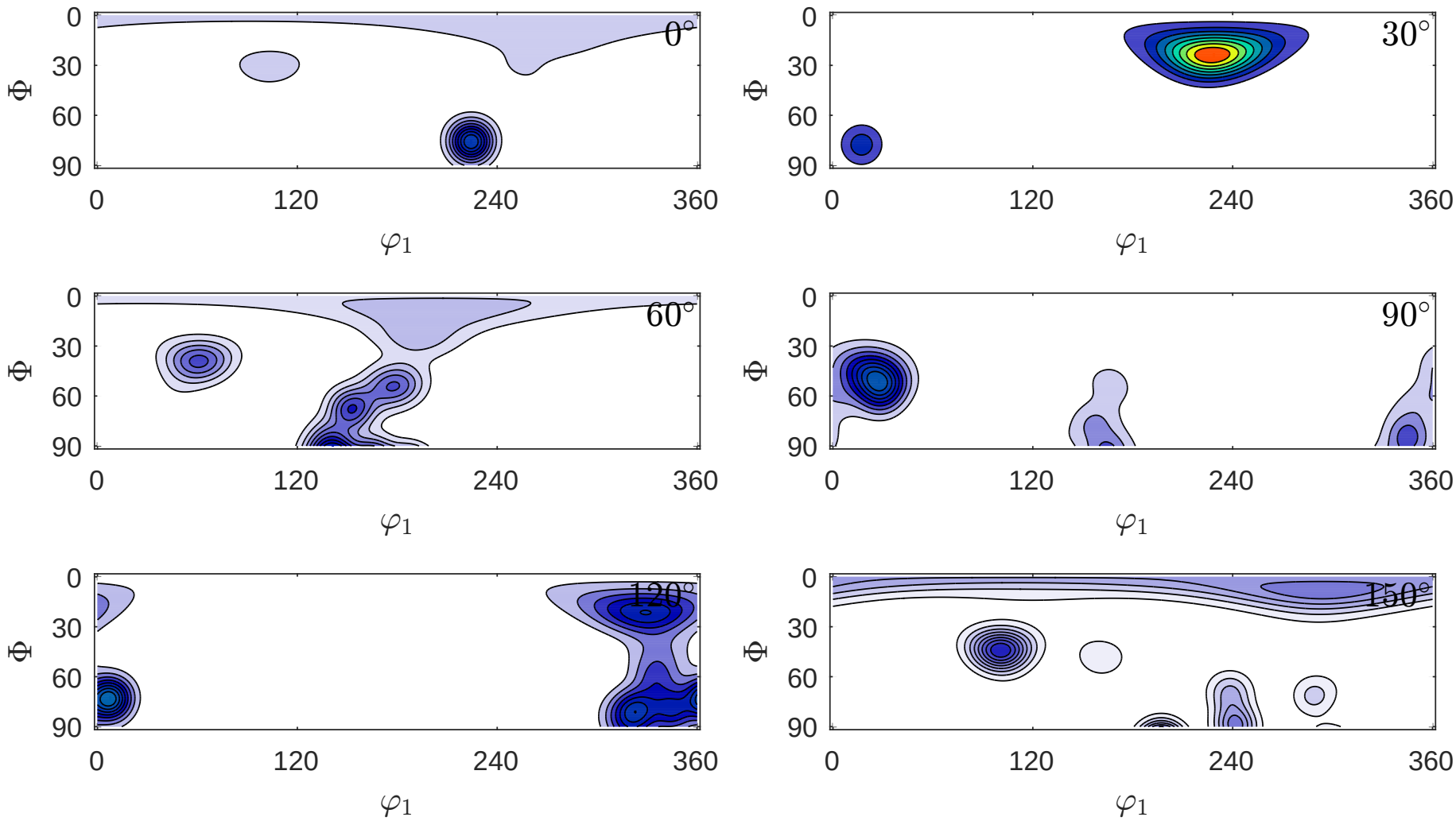
Plotting in Orientation Space

```
plotSection(O,'phi2',(0:30:150)*degree)
```



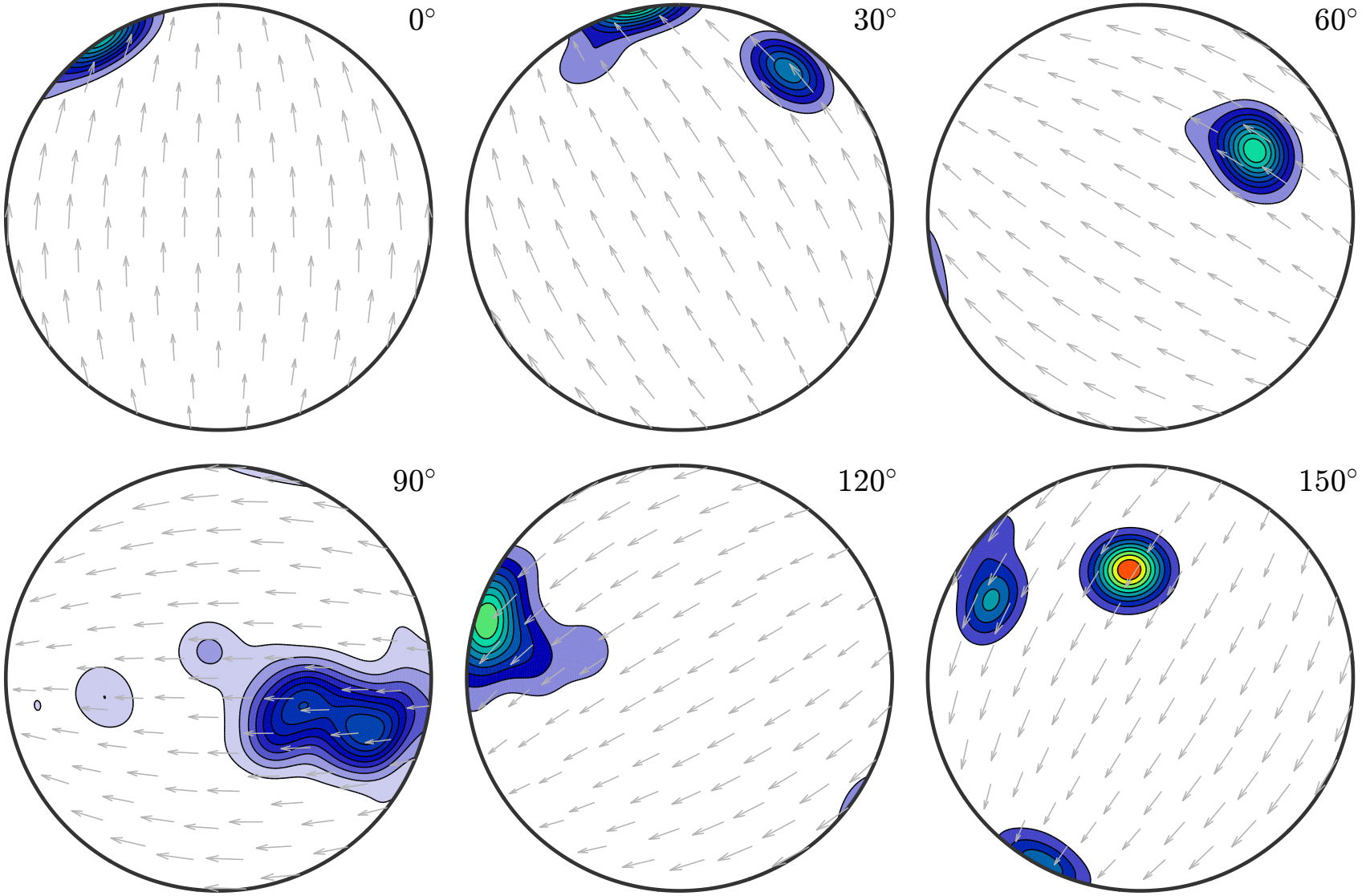
Plotting in Orientation Space

```
plotSection(O,'phi2',(0:30:150)*degree,'contourf')
```



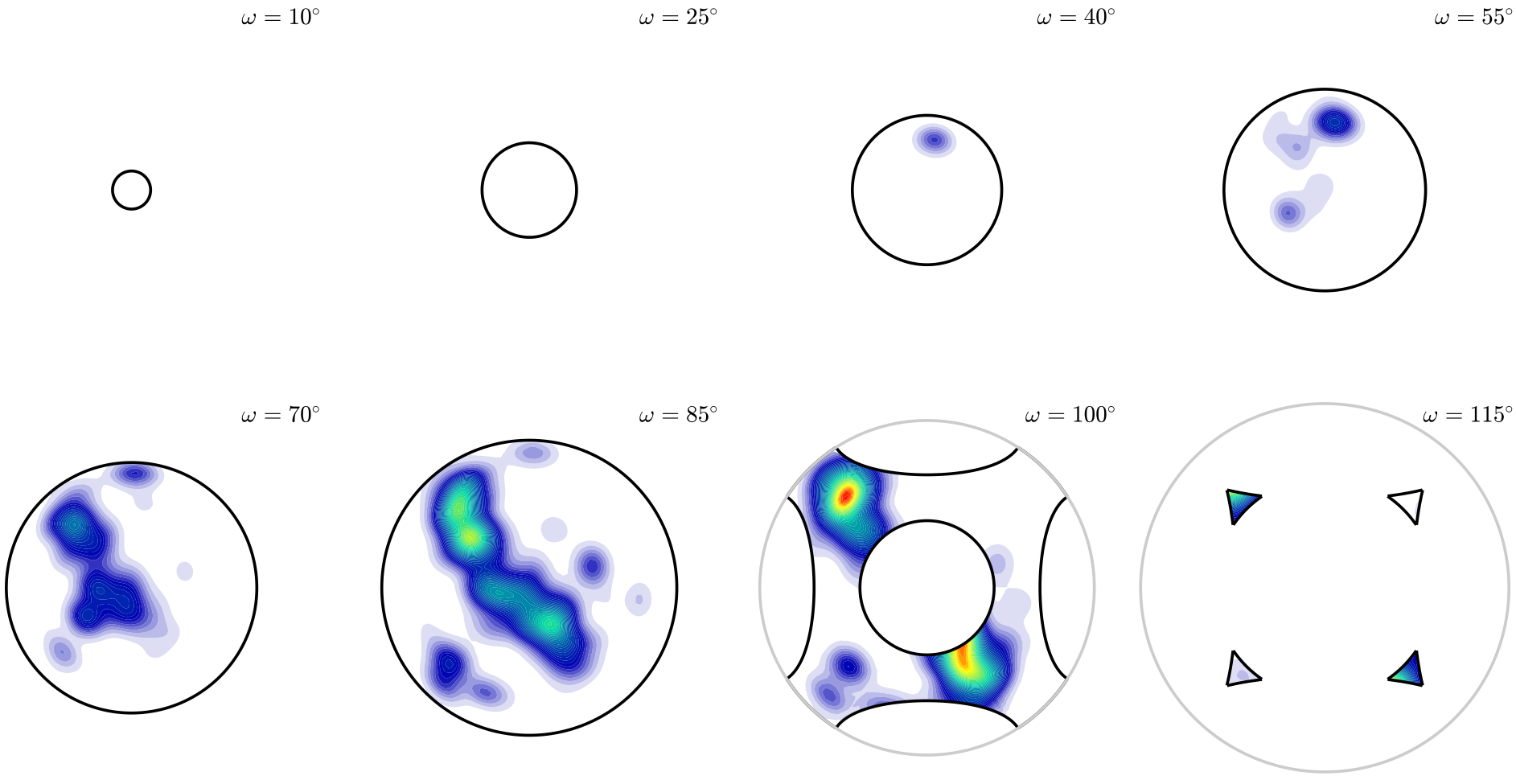
Plotting in Orientation Space

```
plotSection(O, 'sigma',(0:30:150)*degree, 'contourf')
```



Plotting in Orientation Space

```
plotSection(O, 'AxisAngle',(10:15:115)*degree, ...
                'contourf')
```



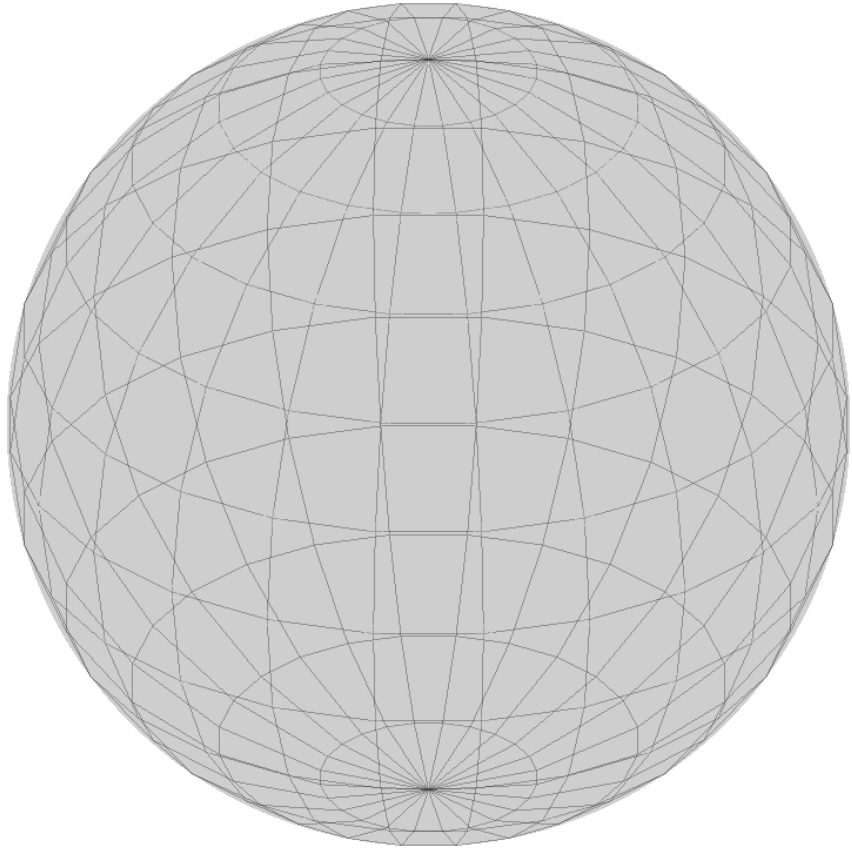
The Orientation Space

```
plot(orientationRegion)
```

```
cs = crystalSymmetry('mmm')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('321')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('432')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

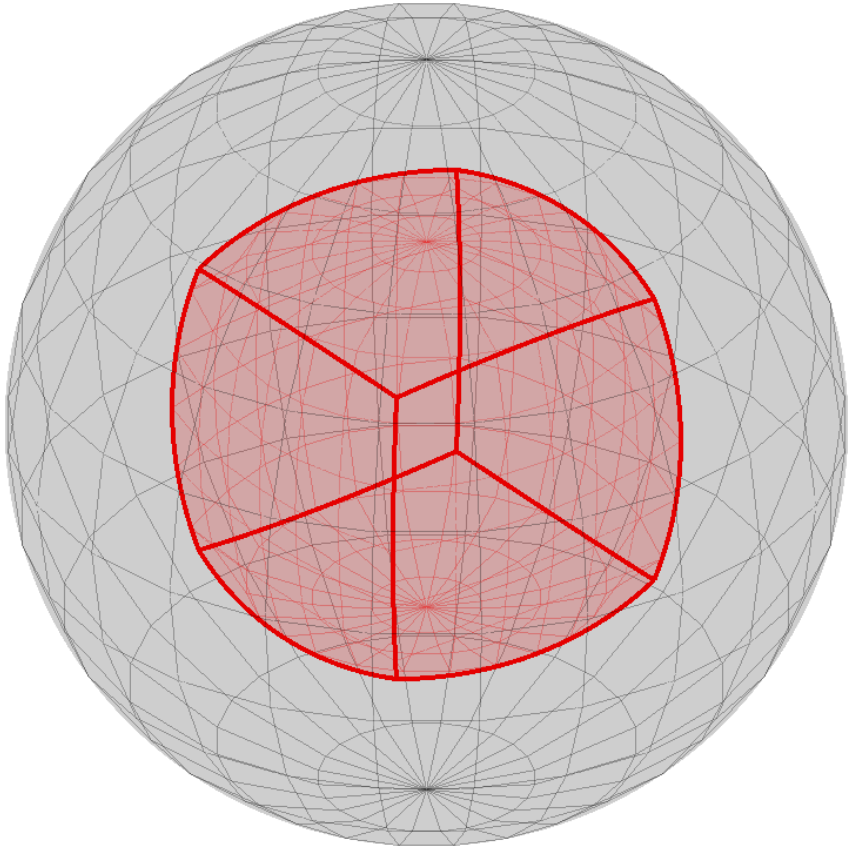


```
oR.V, oR.N, oR.checkInside, oR.axisSector(omega),
oR.maxAngle(axes), oR.minAngle,
oR.calcAxisDistribution, oR.calcAngleDistribution
```

The Orientation Space

```
plot(orientationRegion)
```

```
cs = crystalSymmetry('mmm')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```



```
cs = crystalSymmetry('321')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('432')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
oR.V, oR.N, oR.checkInside, oR.axisSector(omega),
oR.maxAngle(axes), oR.minAngle,
oR.calcAxisDistribution, oR.calcAngleDistribution
```

The Orientation Space

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```

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cs = crystalSymmetry('mmm')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('321')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('432')
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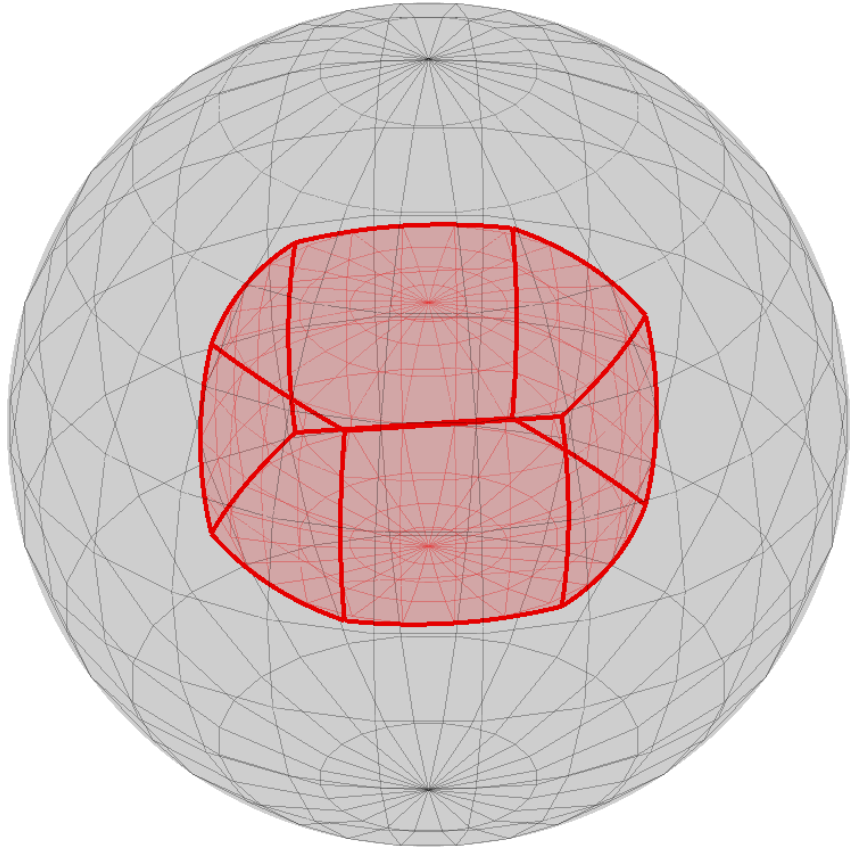
```



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oR.V, oR.N, oR.checkInside, oR.axisSector(omega),
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The Orientation Space

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cs = crystalSymmetry('432')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

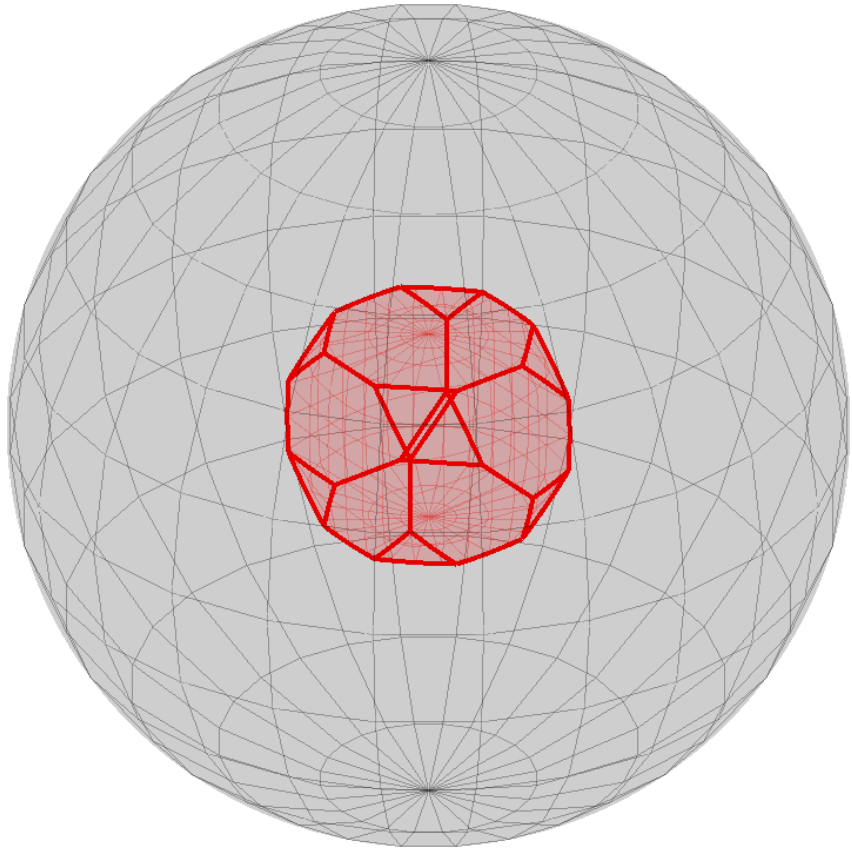

```
oR.V, oR.N, oR.checkInside, oR.axisSector(omega),
oR.maxAngle(axes), oR.minAngle,
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```

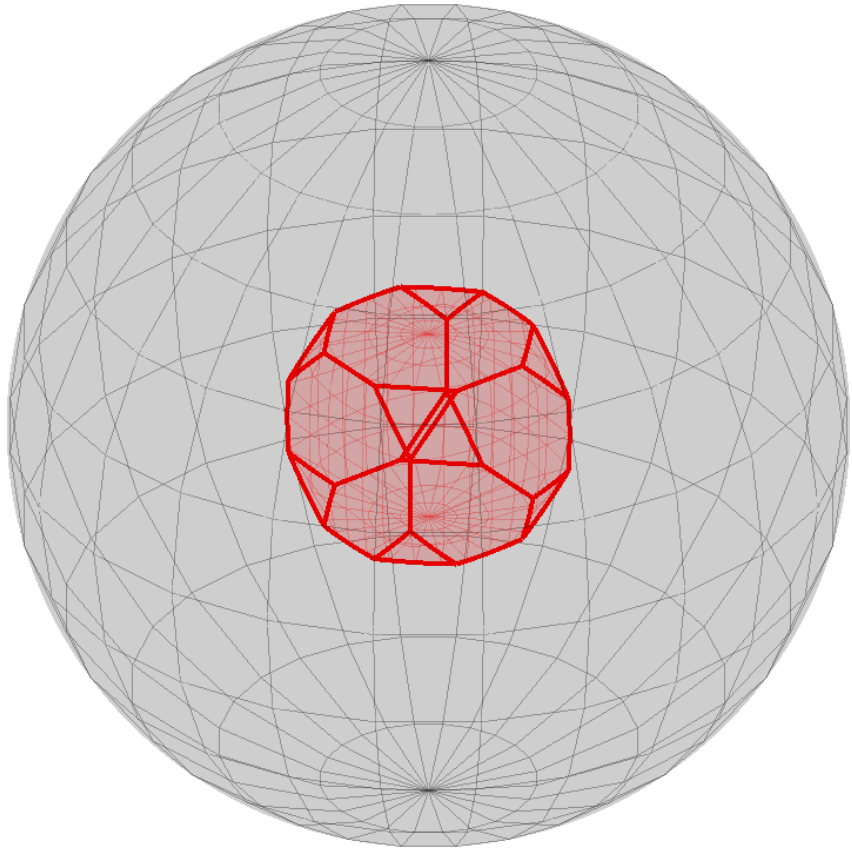
The Orientation Space

```
plot(orientationRegion)
```

```
cs = crystalSymmetry('mmm')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('321')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```

```
cs = crystalSymmetry('432')
oR = cs.fundamentalRegion
plot(oR,'color','r')
```



```
oR.V, oR.N, oR.checkInside, oR.axisSector(omega),
oR.maxAngle(axes), oR.minAngle,
oR.calcAxisDistribution, oR.calcAngleDistribution
```

Operations on Orientations

mean orientation

$$MO = \mathbf{mean}(O)$$

```
MO = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry : Forsterite (mmm)
  specimen symmetry: 1

  Bunge Euler angles in degree
     phi1      Phi     phi2     Inv.
  342.532 68.3179 284.955        0
```

mean orientation spread

$$\mathbf{mean}(\mathbf{angle}(O, MO))./\mathbf{degree}$$

volume portions

$$\mathbf{volume}(O, MO, 10*\mathbf{degree})$$

ODF estimation

$$odf = \mathbf{calcODF}(O, 'halfwidth', 10*\mathbf{degree})$$

Operations on Orientations

mean orientation

```
MO = mean(O)
```

mean orientation spread

```
mean(angle(O, MO))./degree
```

```
ans =

   47.2287
```

volume portions

```
volume(O, MO, 10*degree)
```

ODF estimation

```
odf = calcODF(O,'halfwidth',10*degree)
```

export to ASCII file

```
export(O,'file.txt','degree')
```

Operations on Orientations

mean orientation

```
MO = mean(O)
```

mean orientation spread

```
mean(angle(O, MO))./degree
```

volume portions

```
volume(O, MO, 10*degree)
```

ODF estimation

```
odf = calcODF(O,'halfwidth',10*degree)
```

export to ASCII file

```
export(O,'file.txt','degree')
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export to ASCII file

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Operations on Orientations

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ODF estimation

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odf = calcODF(O,'halfwidth',10*degree)
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export to ASCII file

```
export(O,'file.txt','degree')
```

Fibres

```
cs = crystalSymmetry('432')
ss = specimenSymmetry('222')
o1 = orientation.goss(cs,ss)
o2 = orientation.brass(cs,ss)
f = fibre(o1,o2,'full')

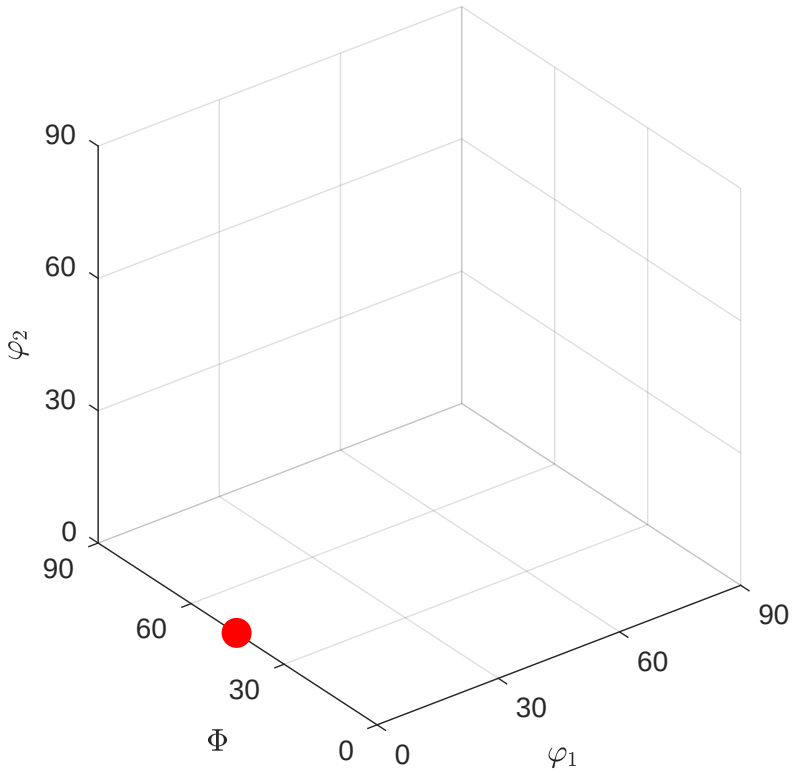
f.symmetrise

f = fibre.beta(cs,ss)

h = Miller(1,1,1,cs)
f = fibre(h,vector3d.Z)

f = fibre.fit(ori)

angle(ori,f)
volume(ori,f,5*degree)
```



Fibres

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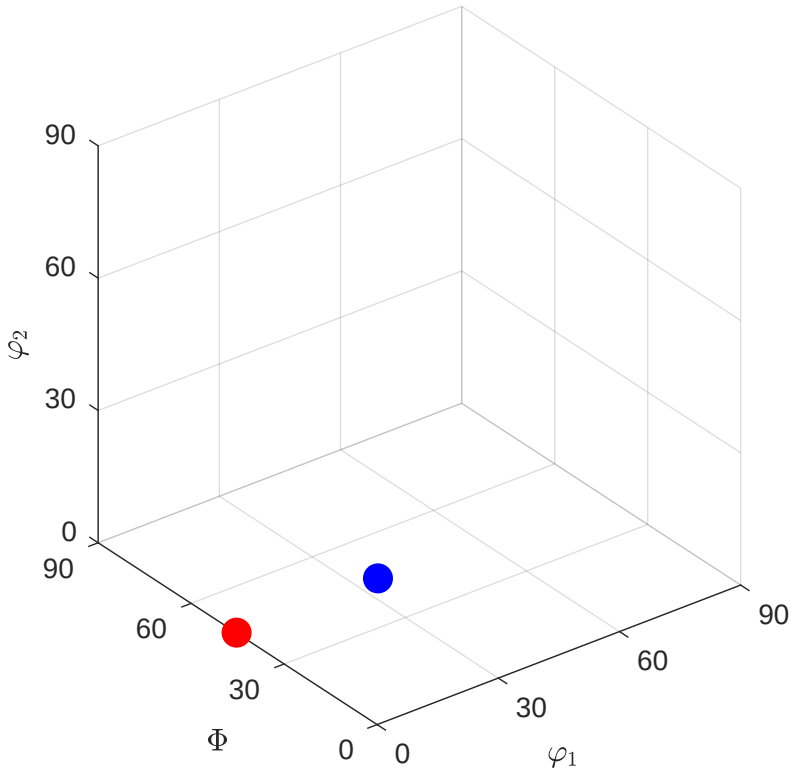


Fibres

```
cs = crystalSymmetry('432')
ss = specimenSymmetry('222')
o1 = orientation.goss(cs,ss)
```

```
o2 = orientation.brass(cs,ss)
```

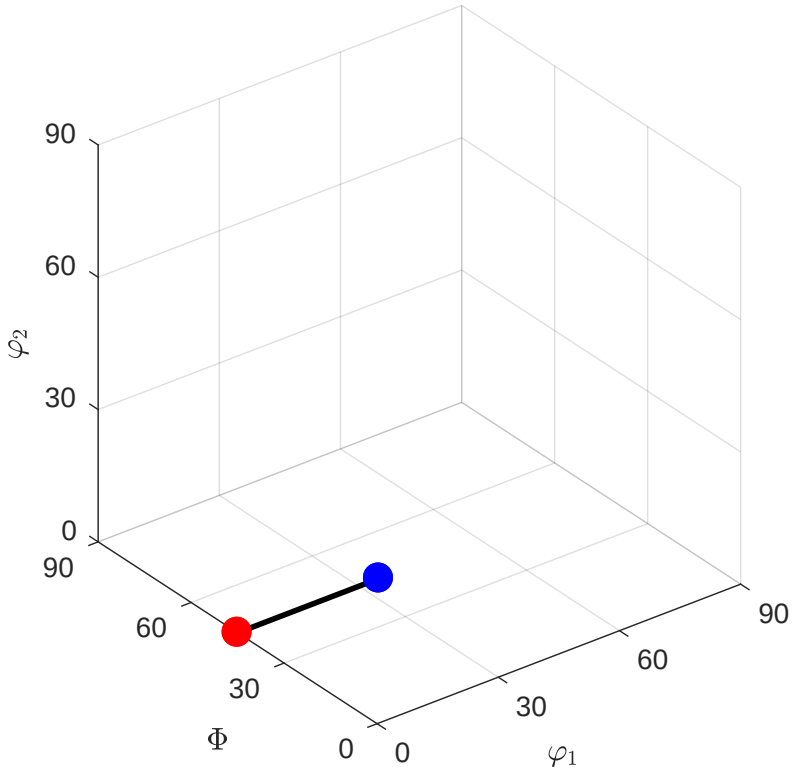
```
f = fibre(o1,o2)
```

```
f = fibre (show methods, plot)
  size: 1 x 1
  crystal symmetry: 432
  specimen symmetry: 222
  o1: (0,45,0)
  o2: (35,45,0)
```

```
f = fibre(o1,o2,'full')
```

```
f.symmetrise
```

```
f = fibre.beta(cs,ss)
```



Fibres

```
cs = crystalSymmetry('432')
ss = specimenSymmetry('222')
o1 = orientation.goss(cs,ss)
```

```
o2 = orientation.brass(cs,ss)
```

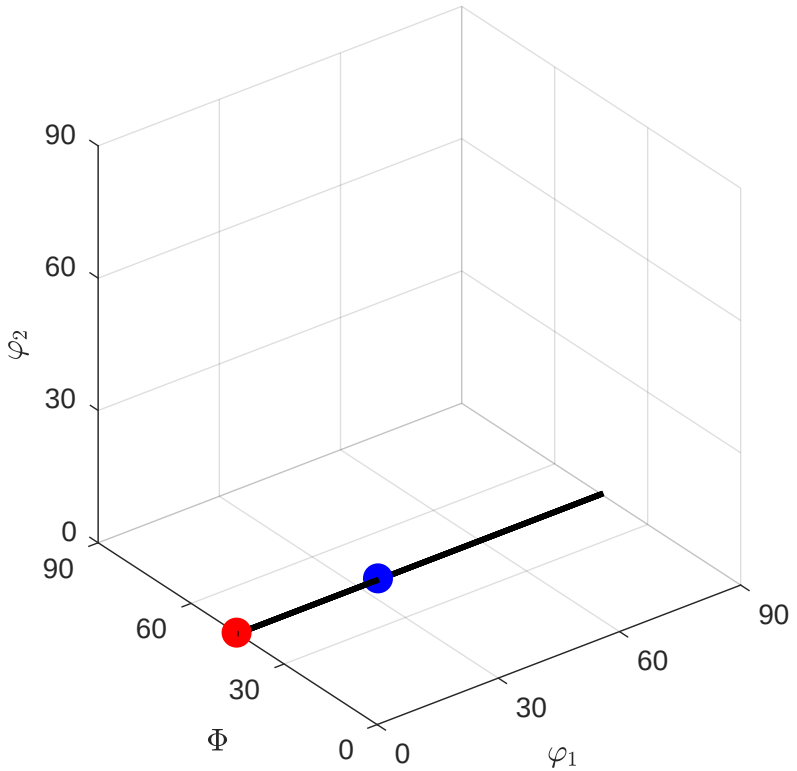
```
f = fibre(o1,o2,'full')
```

```
f = fibre (show methods, plot)
  size: 1 x 1
  crystal symmetry: 432 specimen
  symmetry: 222
  o1: (0,45,0)
  h: (011)
```

```
f.symmetrise
```

```
f = fibre.beta(cs,ss)
```

```
h = Miller(1,1,1,cs)
f = fibre(h,vector3d.Z)
```



Fibres

```
cs = crystalSymmetry('432')
ss = specimenSymmetry('222')
o1 = orientation.goss(cs,ss)
```

```
o2 = orientation.brass(cs,ss)
```

```
f = fibre(o1,o2,'full')
```

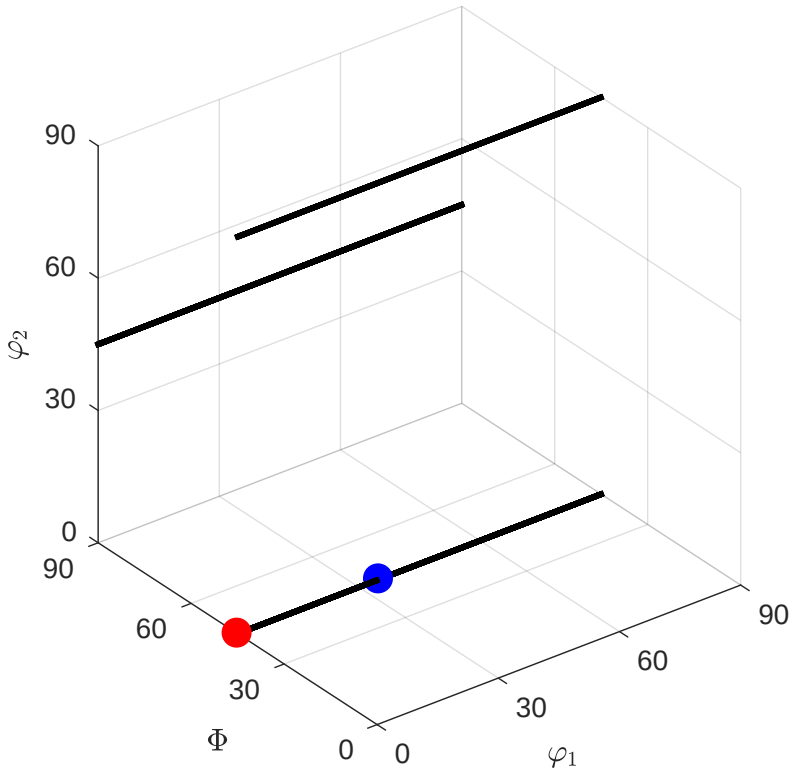
```
f.symmetrise
```

```
f = fibre (show methods, plot)
  size: 12 x 1
  crystal symmetry: 432 specimen
  symmetry: 222
```

```
f = fibre.beta(cs,ss)
```

```
h = Miller(1,1,1,cs)
f = fibre(h,vector3d.Z)
```

```
f = fibre.fit(ori)
```



Fibres

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```
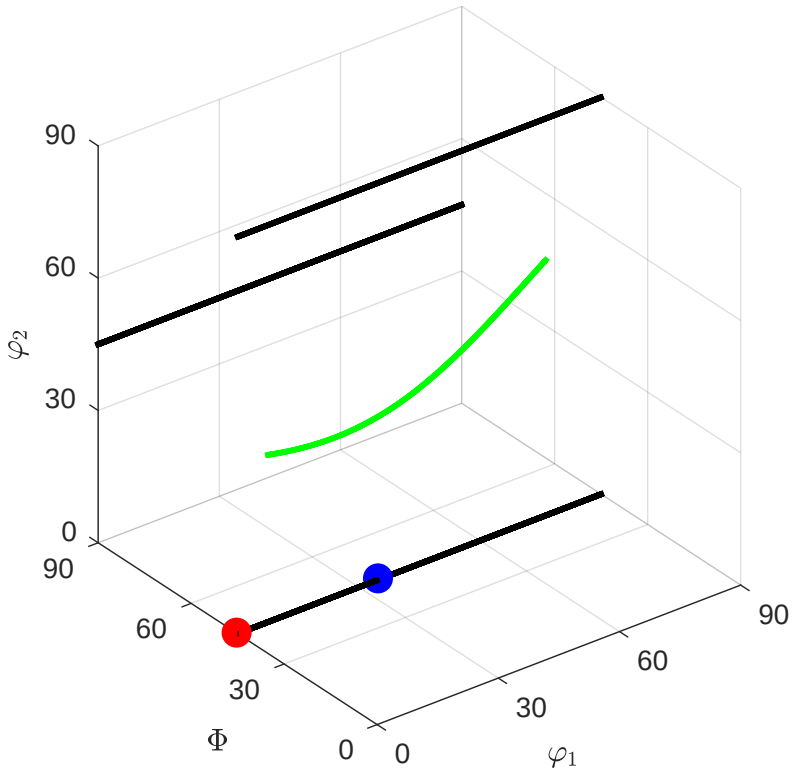

```
angle(ori,f)
volume(ori,f,5*degree)
```



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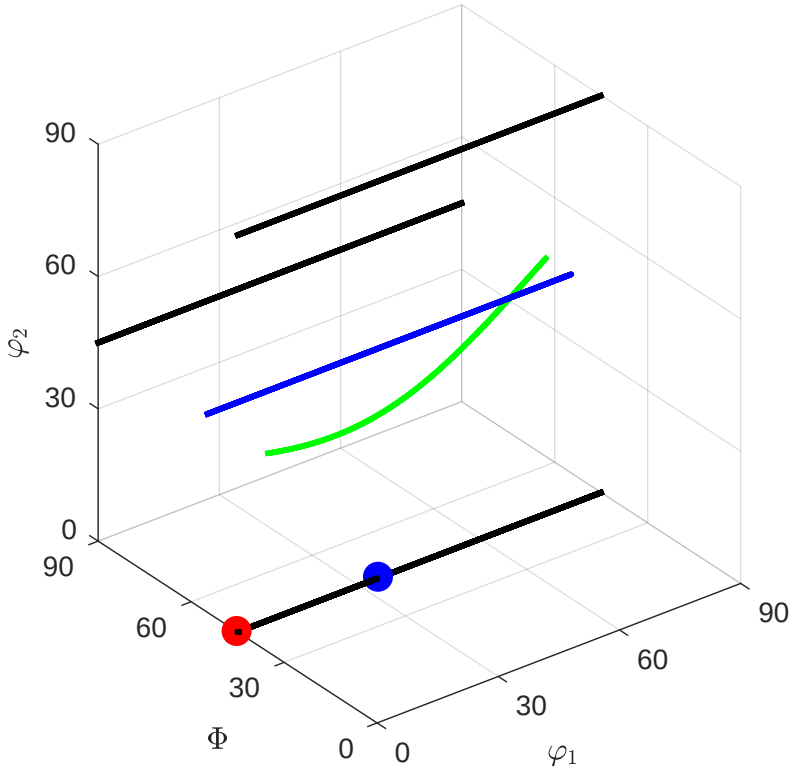
```



Fibres

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```

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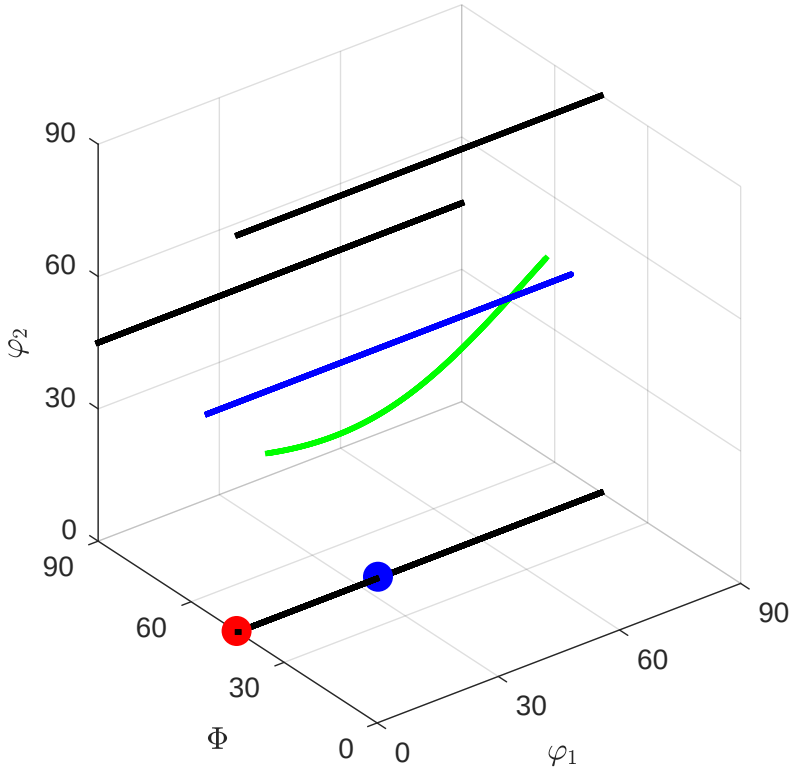

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```

```
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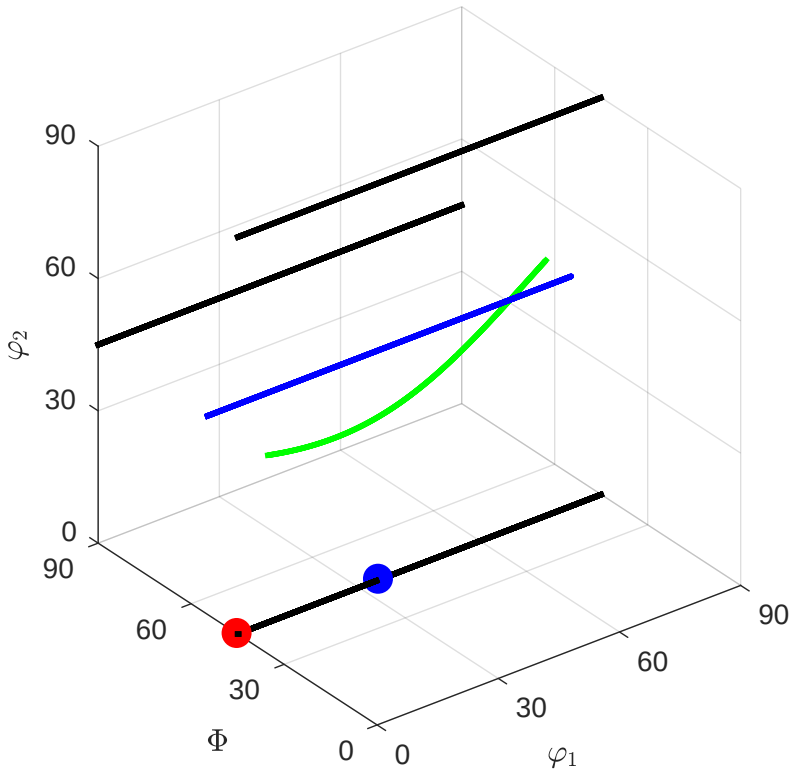
```

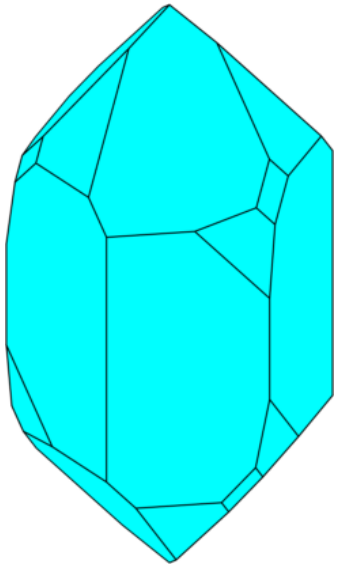


Simple Crystal Shapes

predefined crystal shapes

```
cS = crystalShape.quartz
```

```
cS = crystalShape (show methods, plot)
 mineral: Quartz (321, X||a*,Y||b,Z||c*)
 vertices: 56
 faces: 30
```



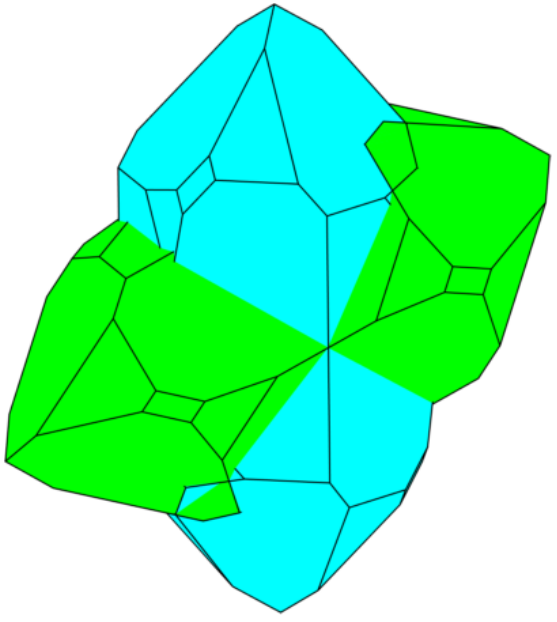
Simple Crystal Shapes

predefined crystal shapes

```
cS = crystalShape.quartz
```

illustrate orientation relationships

```
mori = orientation.byAxisAngle(...
   Miller(1,0,-1,1,cs),87*degree)
plot(mori * cS,'facecolor','green')
```



Simple Crystal Shapes

predefined crystal shapes

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```
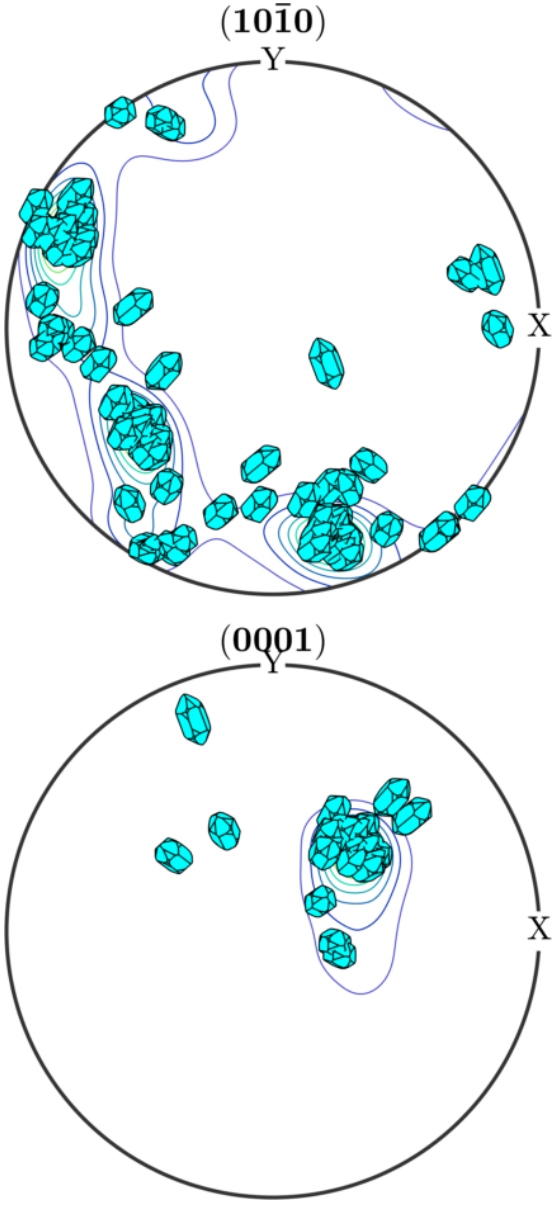

illustrate orientation relationships

```
mori = orientation.byAxisAngle(...
   Miller(1,0,-1,1,cs),87*degree)
plot(mori * cS,'facecolor','green')
```

annotate to pole figures

```
h = Miller({1,0,-1,0},{0,0,0,1},cs)
plotPDF(odf,h,'contour')
plot(ori,0.3*ori*cS,'add2all')
```



Simple Crystal Shapes

predefined crystal shapes

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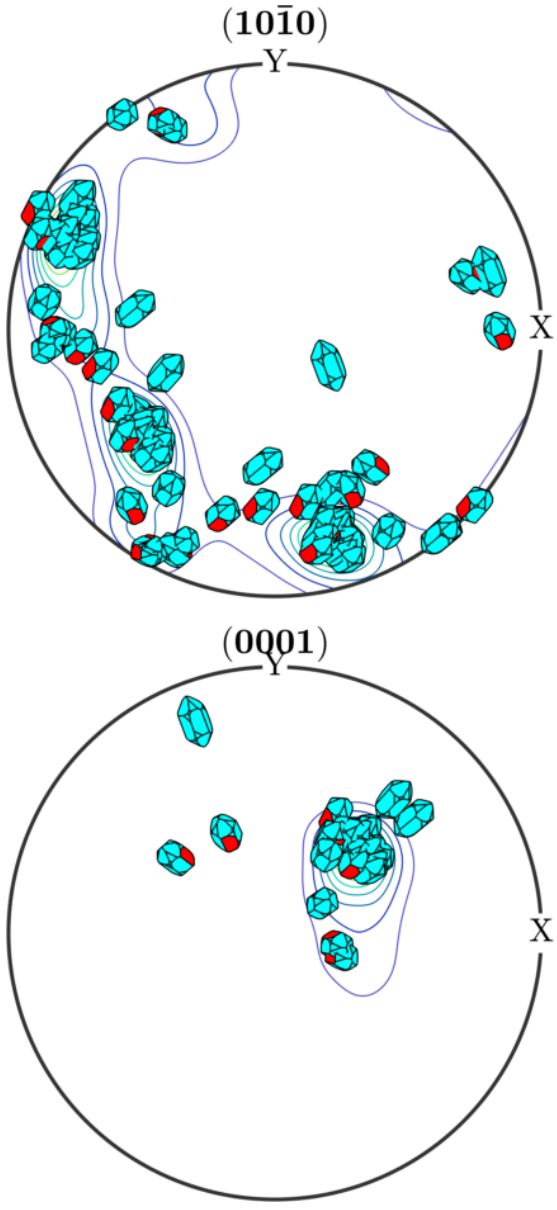
```
mori = orientation.byAxisAngle(...
   Miller(1,0,-1,1,cs),87*degree)
plot(mori * cS,'facecolor','green')
```

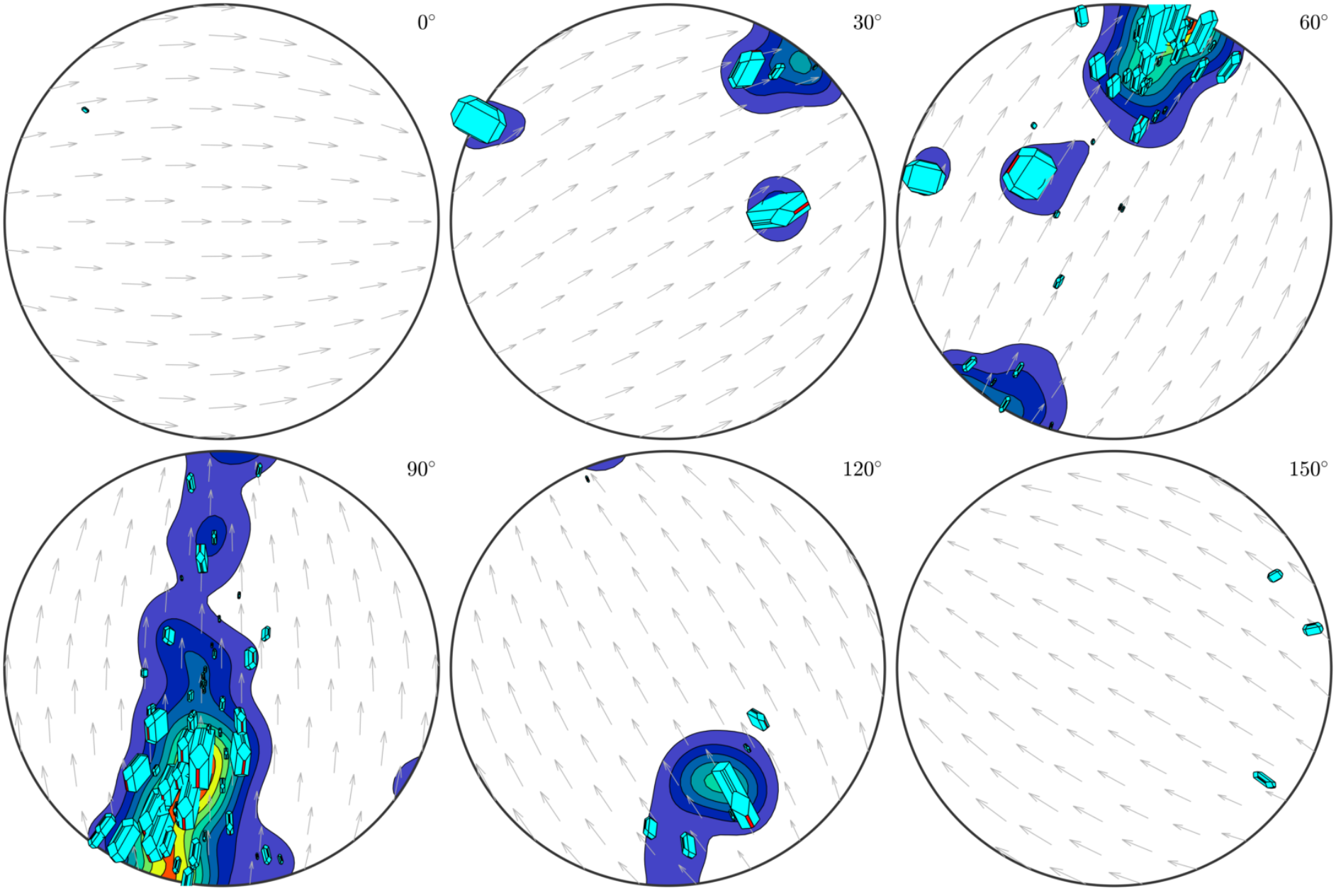
annotate to pole figures

```
h = Miller({1,0,-1,0},{0,0,0,1},cs)
plotPDF(odf,h,'contour')
plot(ori,0.3*ori*cS,'add2all')
```

highlight specific faces

```
plot(ori,0.3*ori*cS(h(1)),'add2all')
```




0°
30°
60°
90°
120°
150°

The Code

```
odf = calcODF(ebsd('Fo').orientations)
plotSection(odf,'sigma')

% consider large Forsterite grains only
grains = calcGrains(ebsd)
lg = grains(grains.area > 50000); lg = lg('Fo')
ori = lg.meanOrientation;

scaling = 0.5 * sqrt(lg.area/max(lg.area));
cS = scaling .* (ori .* cS);

plot(ori,cS,'add2all')

h = Miller({0,0,1},{1,0,0},cS.CS);
plot(ori,cS(h(1)),'add2all','faceColor','red')
plot(ori,cS(h(2)),'add2all','faceColor','green')
```