

Crystal Geometry

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

Three dimensional vectors are given by their coordinates with respect to an 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)
```

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

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

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

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

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

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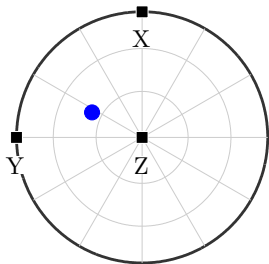
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```
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```
plotx2north , plotzOutOfPlane  
plot(r)
```



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

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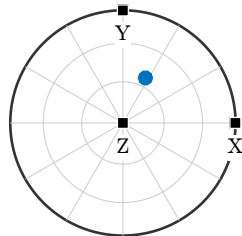
$$\vec{r} = x \cdot \vec{X} + y \cdot \vec{Y} + z \cdot \vec{Z}$$

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

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

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

```
plotx2east , plotzOutOfPlane  
plot(r)
```



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

Defining vectors

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

```
r = vector3d( 'theta ', theta , 'rho ', rho )
```

predefined vectors

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

combine vectors

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

importing vectors

```
r = loadVector3d( 'file ', 'ColumnNames ', { 'x ', 'y ', 'z ' } )
```

Defining vectors

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```

```
r = vector3d (show methods, plot)
size: 1 x 3
x y z
1 0 0
0 1 0
1 1 1
```

importing vectors

```
r = loadVector3d('file', 'ColumnNames', {'x', 'y', 'z'})
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```

importing vectors

```
r = loadVector3d( 'file ', 'ColumnNames', { 'x ', 'y ', 'z ' })
```

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

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
```

extract properties

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

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extract properties

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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

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r = vector3d (show methods, plot)
  size: 1 x 1
  x y z
  0 0 1
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single out the second and the fourth vector

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

single out vectors by a logical condition

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

The show techniques apply also to lists of rotation / orientations

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

single out vectors by a logical condition

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r(r.x>0)
```


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```
r(2)
```

single out the second and the fourth vector

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

single out vectors by a logical condition

```
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

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```
r = vector3d([0 0 1 1],[1 0 1 1],[1 1 1 0]);
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replace the second vector by another vector

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

remove the second vector completely

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replace the second vector by another vector

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```

remove the second vector completely

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

```
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
```

Changing Vectors

consider again the list of vectors

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

replace the second vector by another vector

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r(2) = vector3d.Y
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```
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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

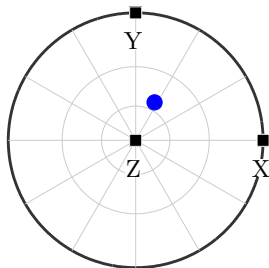
```
plot(vector3d(1,1,1), 'upper');  
hold on  
plot(vector3d(1,2,3), 'label', 'B');  
plot(vector3d(-1,2,1), 'label', 'A');  
hold off
```

scatter plots

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

contour plots

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



Plotting Vectors

spherical projections: earea, edist, eangle

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plot(r, 'projection', 'earea', 'upper')
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combined plots

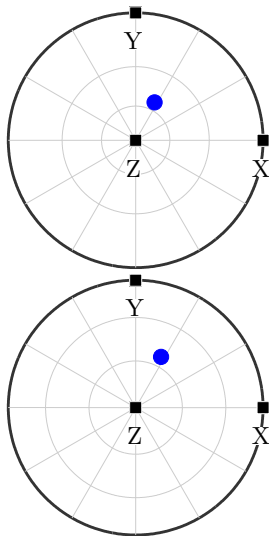
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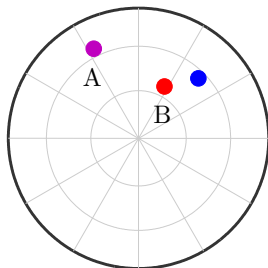
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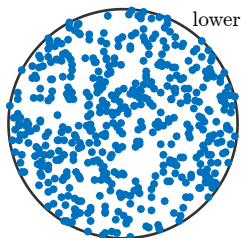
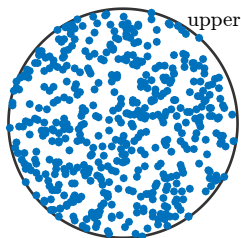
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Plotting Vectors

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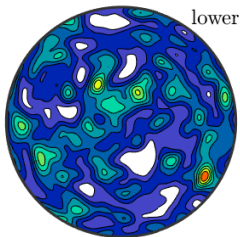
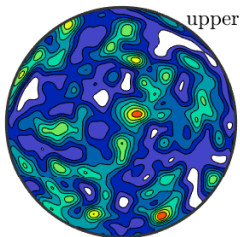
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Data Plots

colorize vectors by value

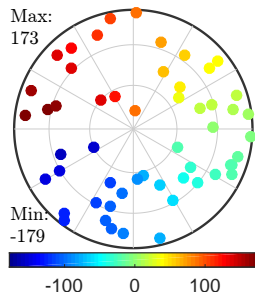
```
v = vector3d.rand(100)
scatter(v, v.rho./degree)
mtexColorbar southoutside
mtexColorMap jet
```

colorize by RGB triples

```
oM = ipdfHSVOrientationMapping
scatter(v, oM.Miller2color(v))
```

visualize directions

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



Data Plots

colorize vectors by value

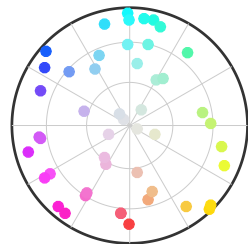
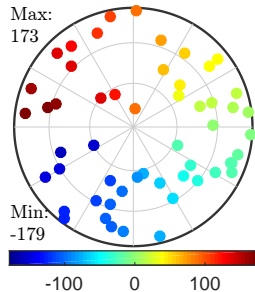
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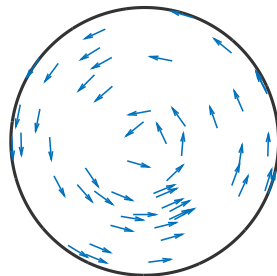
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```



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
```

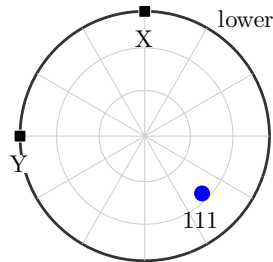
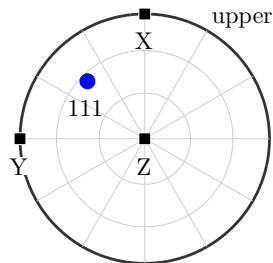
Then r and $-r$ represent the same axis

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

The angle to an axis is always less than 90°

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

The option **antipodal** in density estimation



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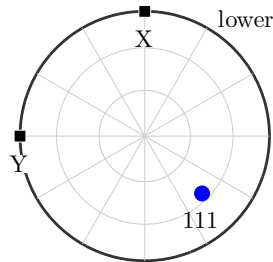
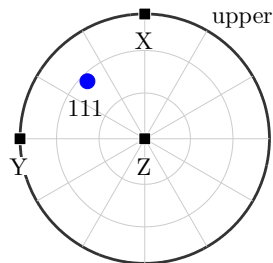
```
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```

```
1
```

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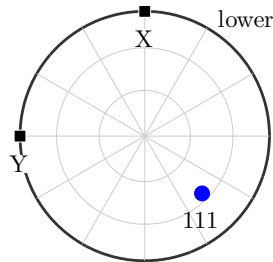
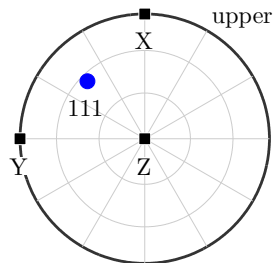
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```
angle(r, -vector3d.X) / degree
```

```
54.7
```

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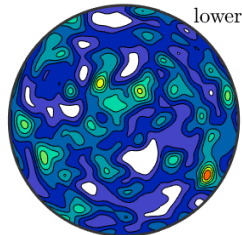
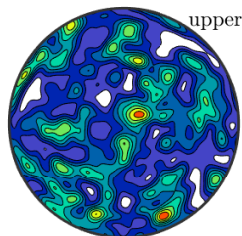
```
angle(r, -vector3d.X) / degree
```

The option **antipodal** in density estimation

```
r = vector3d.rand(1000)
```

```
sF = calcDensity(r)
```

```
contourf(sF)
```



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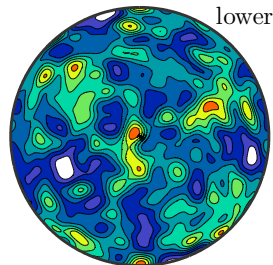
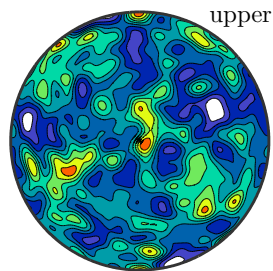
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The angle to an axis is always less than 90°

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

The option **antipodal** in density estimation

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



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

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

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

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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

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

Euler Angles

Most commonly, rotations are given by Bunge Euler angles.

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

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

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

Euler Angles

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```
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```
size: 1 x 1
```

```
Roe Euler angles in degree
```

```
Psi Theta Phi Inv.
```

```
10 20 30 0
```

Other Ways to Define a Rotation

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

```
R = rotation( 'axis', vector3d.X, 'angle', 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( 'matrix', A )
```

or by quaternions

```
R = rotation( 'quaternion', a, b, c, d )
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or by quaternions

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

Basic Calculations

rotate a vector

```
R = rotation('axis', vector3d.X, 'angle', -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)
```

Basic Calculations

rotate a vector

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

the inverse rotation

```
inv(R)
```

```
ans = rotation (show methods, plot)  
size: 1 x 1  
  
Bunge Euler angles in degree  
phi1 Phi phi2 Inv.  
0 45 0 0
```

combine rotations

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R * inv(R)
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Bunge Euler angles in degree  
phi1 Phi phi2 Inv.  
0 0 0 0
```

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Basic Calculations

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inv(R)
```

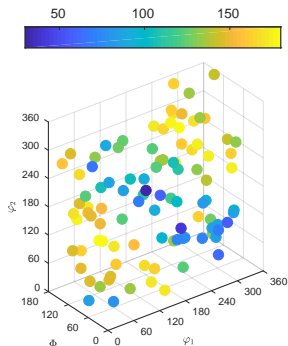
combine rotations

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

plotting

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

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



Basic Calculations

rotate a vector

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

the inverse rotation

```
inv(R)
```

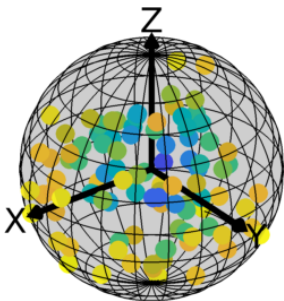
combine rotations

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

plotting

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

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



Improper Rotations

An improper rotation is a rotation followed by an inversion

```
I = -rotation('Euler', 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])
```

Improper Rotations

An improper rotation is a rotation followed by an inversion

```
I = -rotation('Euler', 10*degree, 20*degree, 30*degree)
```

reflections

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

```
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

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

Improper Rotations

An improper rotation is a rotation followed by an inversion

```
I = -rotation('Euler', 10*degree, 20*degree, 30*degree)
```

reflections

```
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

```
I = -rotation('Euler', 10*degree, 20*degree, 30*degree)
```

reflections

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

angles between proper and improper rotations

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

check for improper rotations

```
I.isImproper
```

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

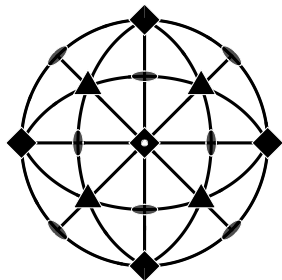
```
rotation(crystalSymmetry('222'))
```

import data from crystal information files

```
CS = loadCIF('Quarz.cif')
```

```
CS = loadPHL('minerals.phl')
```

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.

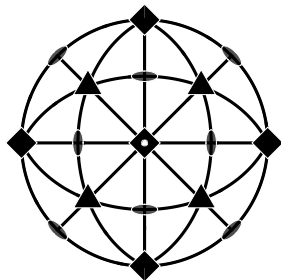
```
CS = crystalSymmetry('m-3m')
```

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 data from crystal information files

```
CS = loadCIF('Quarz.cif')
```


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'))
```

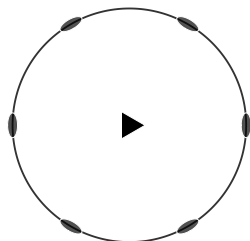
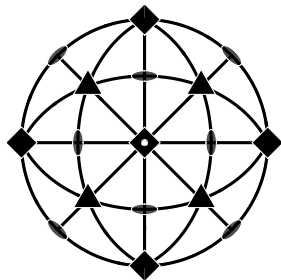
import data from crystal information files

```
CS = loadCIF('Quarz.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*
```

```
CS = loadPHL('minerals.phl')
```



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'))
```

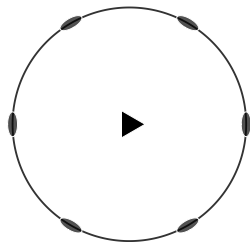
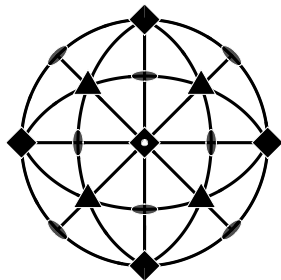
import data from crystal information files

```
CS = loadCIF('Quarz.cif')
```

```
CS = loadPHL('minerals.phl')
```

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

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



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 data from crystal information files

```
CS = loadCIF('Quarz.cif')
```

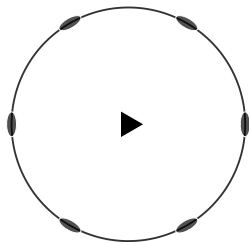
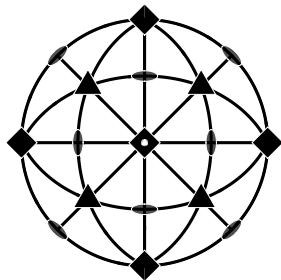
```
CS = loadPHL('minerals.phl')
```

switch to Laue / purely rotational group

```
CS.Laue
```

```
CS.properGroup
```

```
CS.properSubGroup
```



Vectors

oooooooo

Rotations

ooooo

Crystal Symmetries

o●ooo

Miller Indices

ooo

Orientations

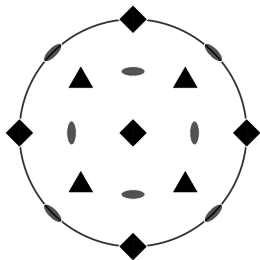
oooooooo

Fibres

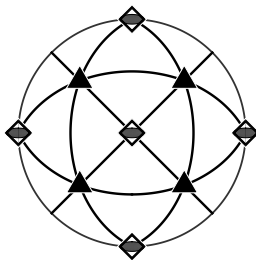
o

Crystal Shapes

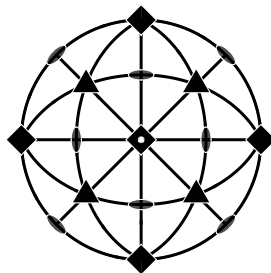
ooo



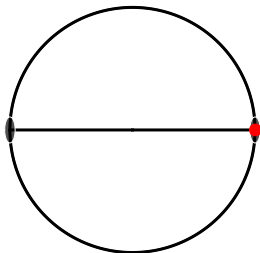
432



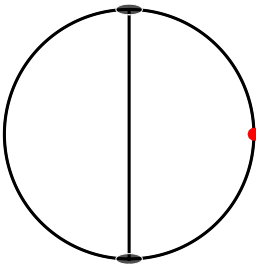
$\bar{4}3m$



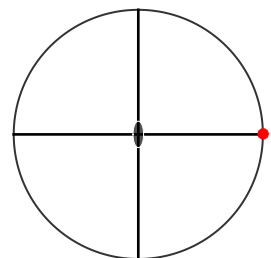
$m\bar{3}m$



2mm



m2m



mm2

Vectors

oooooooo

Rotations

ooooo

Crystal Symmetries

oo●oo

Miller Indices

ooo

Orientations

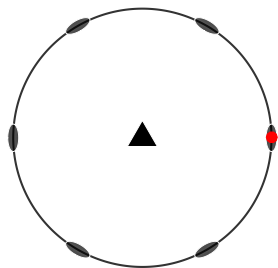
ooooooo

Fibres

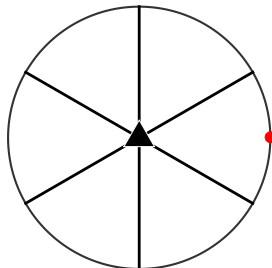
o

Crystal Shapes

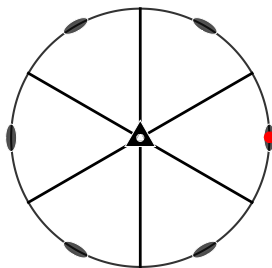
ooo



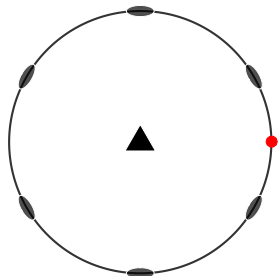
321



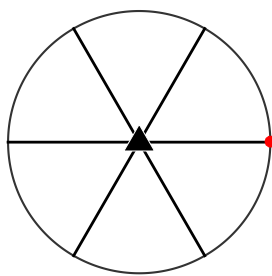
3m1



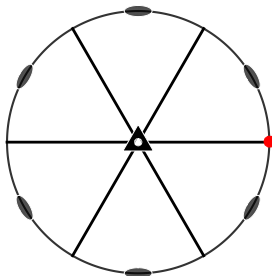
$\bar{3}m1$



312



31m



$\bar{3}1m$

Plotting conventions

directions with respect to the sample frame → `vector3d`

pole figures, field tensors, directional grain properties

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

directions with respect to the crystal frame → Miller

inverse pole figures, misorientation axis, ip color keys, matter tensors

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

Plotting conventions

directions with respect to the sample frame → `vector3d`

pole figures, field tensors, directional grain properties

**`plotx2east` , `plotx2north` , `plotx2west` , `plotx2south`
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directions with respect to the crystal frame → Miller

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`plotb2east` , `plotb2north` , `plotb2west` , `plotb2south`**

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])

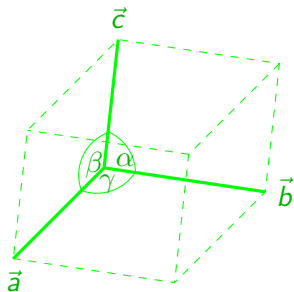
The axes of the reciprocal lattice are defined orthogonal to \vec{a} , \vec{b} , \vec{c} , i.e.

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

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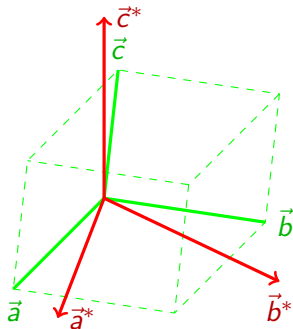
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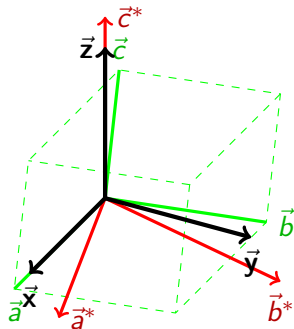
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We will need also an orthogonal coordinate system $(\vec{x}, \vec{y}, \vec{z})$ fixed to the crystal.

There are different conventions.



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

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] )
```

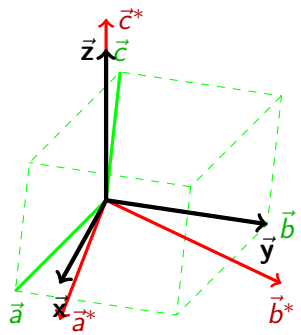
The axes of the reciprocal lattice are defined orthogonal to $\vec{a}, \vec{b}, \vec{c}$, i.e.

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

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

There are different conventions.



```
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

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.

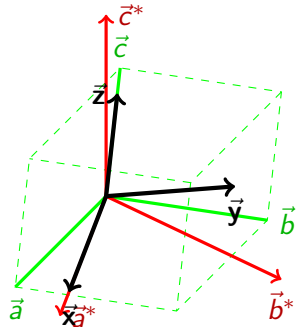
```
C = crystalSymmetry( '1', [a b c], [alpha beta gamma] )
```

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.

```
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)
```

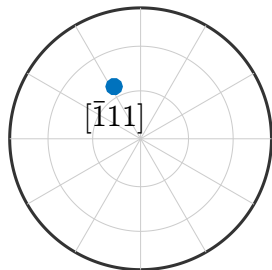
```
size: 1 x 1
```

```
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**

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

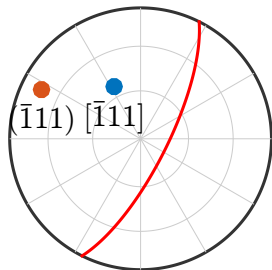
```
CS = crystalSymmetry( 'mmm', [1 2 3] )
m  = Miller( -1, 1, 1, CS, 'uvw' )
```

A direction in reciprocal coordinates

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

```
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' )
```

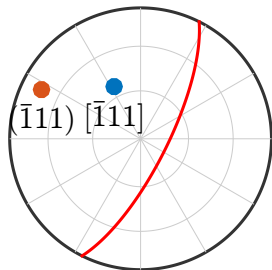
A direction in reciprocal coordinates

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

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

A direction in the orthogonal coordinate system

```
m = Miller( vector3d.X, CS )
```

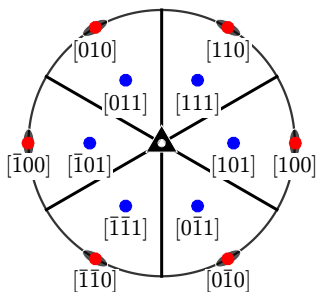
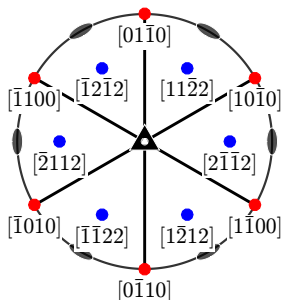
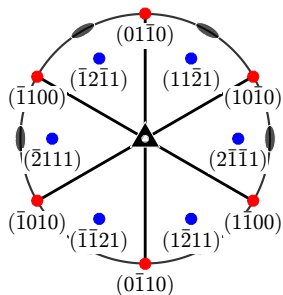


```
plot( m, 'labeled' )
```

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

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


Trigonal and Hexagonal Symmetries



define 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, 'UTW')
```

```
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 = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

```
ans = Miller (show methods, plot)
size: 6 x 1
mineral: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
h 1 -2 1 1 -2 1
k 1 1 -2 -2 1 1
i -2 1 1 1 1 -2
l 1 1 1 1 -1 -1 -1
```

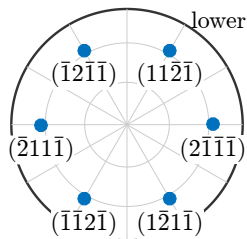
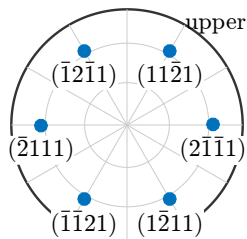
Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

```
m.dispStyle = 'UTW'
```

```
round(m)
```

Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```



Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

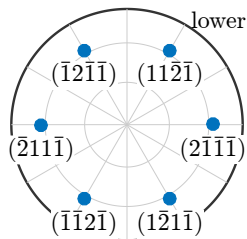
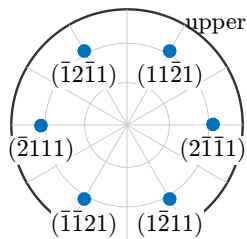
```
m.dispStyle = 'UTW'
```

```
m = Miller (show methods, plot)
size: 6 x 1
mineral: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
U 0.0828
V 0.0828
T -0.1655
W 0.1027
```

```
round(m)
```

Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```



Calculating with Crystal Directions

Find all symmetrically equivalent directions

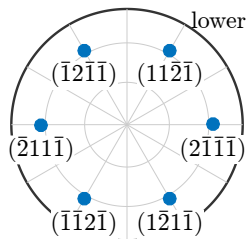
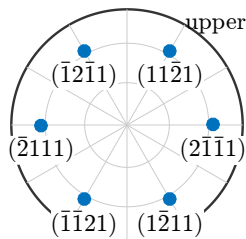
```
CS = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

```
m.dispStyle = 'UTW'
```

```
round(m)
```

```
ans = Miller (show methods, plot)
  size: 6 x 1
  mineral: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
  U 4
  V 4
  T -8
  W 5
```



Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```

Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

```
m.dispStyle = 'UTW'
```

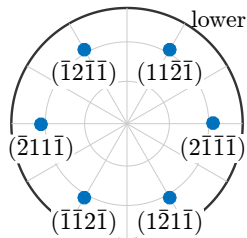
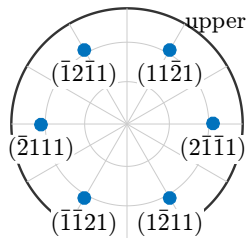
```
round(m)
```

Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```

```
m.dspacing % d-spacing of planes
```

angle modulo symmetry



Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

```
m.dispStyle = 'UTW'
```

```
round(m)
```

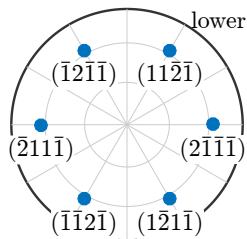
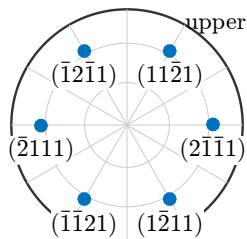
Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```

```
m.dspacing % d-spacing of planes
```

angle modulo symmetry

```
angle(m1,m2) / degree
```



Calculating with Crystal Directions

Find all symmetrically equivalent directions

```
CS = loadCIF('quartz')
m = Miller(1,1,-2,1,CS,'hkil')
symmetrise(m)
```

Change from reciprocal coordinate system to \vec{a} , \vec{b} , \vec{c}

```
m.dispStyle = 'UTW'
```

```
round(m)
```

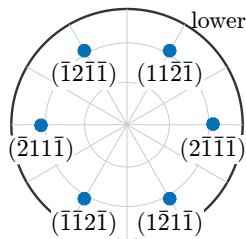
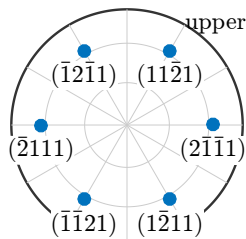
Access the coordinates and properties

```
m.U, m.hkl, m.uvw, m.UTW
```

```
m.dspacing % d-spacing of planes
```

angle modulo symmetry

```
angle(m1,m2,'noSymmetry') / degree
```



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.,

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

The coordinate transform \mathbf{O} with

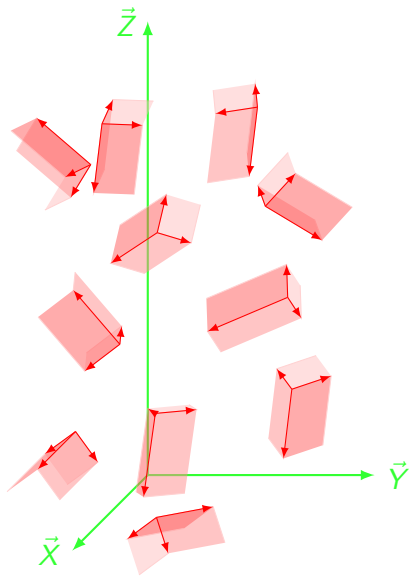
$$(r_1, r_2, r_3)^t = \mathbf{O} (h_1, h_2, h_3)^t$$

is called **crystal orientation**.

Bunge specimen \rightarrow crystal

MTEX crystal \rightarrow specimen

Orientation \mathbf{O} is well defined only modulo crystal symmetry.



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.,

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

The coordinate transform \mathbf{O} with

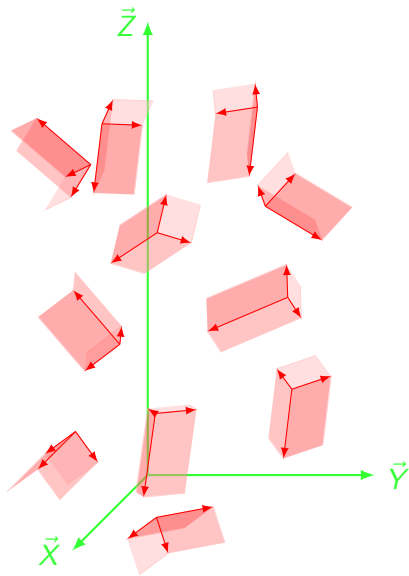
$$(r_1, r_2, r_3)^t = \mathbf{O} (h_1, h_2, h_3)^t$$

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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.,

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

The coordinate transform \mathbf{O} with

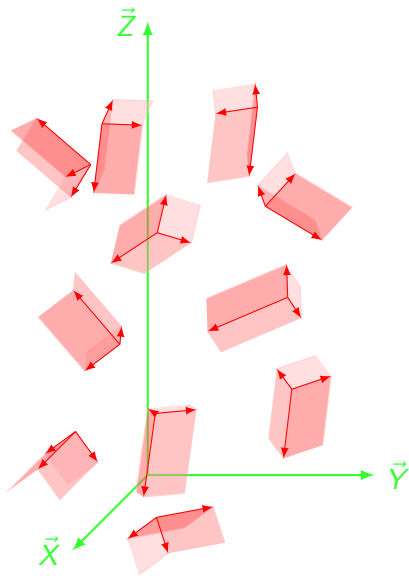
$$(r_1, r_2, r_3)^t = \mathbf{O} (h_1, h_2, h_3)^t$$

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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.,

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

The coordinate transform \mathbf{O} with

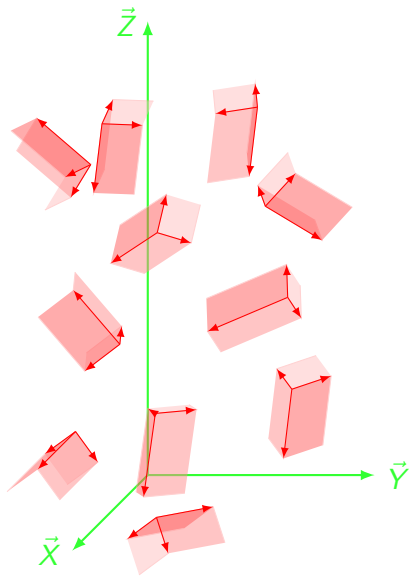
$$(r_1, r_2, r_3)^t = \mathbf{O} (h_1, h_2, h_3)^t$$

is called **crystal orientation**.

Bunge specimen \rightarrow crystal

MTEX crystal \rightarrow specimen

Orientation \mathbf{O} is well defined only modulo crystal symmetry.



Defining Orientations

define an orientation by Euler angles

```
CS = crystalSymmetry( '321' )  
SS = specimenSymmetry( '1' )  
O = orientation( 'Euler', 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  
Psi Theta Phi Inv.  
10 5 0 0
```

import orientations

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

define orientations by Miller indices

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

Defining Orientations

define an orientation by Euler angles

```
CS = crystalSymmetry( '321 ' )  
SS = specimenSymmetry( '1 ' )  
O = orientation( 'Euler', 10*degree, 5*degree, 0, CS, SS)
```

import orientations

```
O = loadOrientation( '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( 'Miller', [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 an orientation by Euler angles

```
CS = crystalSymmetry( '321 ' )  
SS = specimenSymmetry( '1 ' )  
O = orientation( 'Euler', 10*degree, 5*degree, 0, CS, SS)
```

import orientations

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

define orientations by Miller indices

```
O = orientation( 'Miller', [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 an orientation by Euler angles

```
CS = crystalSymmetry( '321 ' )  
SS = specimenSymmetry( '1 ' )  
O = orientation( 'Euler', 10*degree, 5*degree, 0, CS, SS)
```

import orientations

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

define orientations by Miller indices

```
O = orientation( 'Miller', [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('axis',vector3d.Z,'angle',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

inv(O) * r

change specimen coordinates

```
R = rotation('axis',vector3d.Z,'angle',90*degree)
O2 = R * O1
```

Bunge interchange order of multiplication

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('axis',vector3d.Z,'angle',90*degree)  
O2 = R * O1
```

Bunge interchange order of multiplication

Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

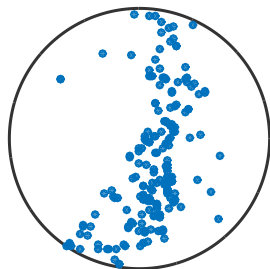
```
plotPDF(O, h, 'contourf')
```

specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

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

```
plotIPDF(O, v, 'contourf')
```



Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

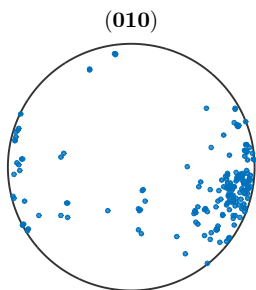
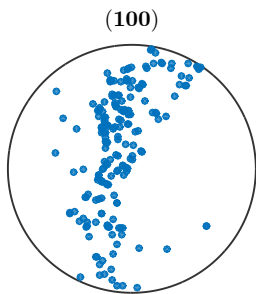
```
plotPDF(O, h, 'contourf')
```

specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

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

```
plotIPDF(O, v, 'contourf')
```



Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

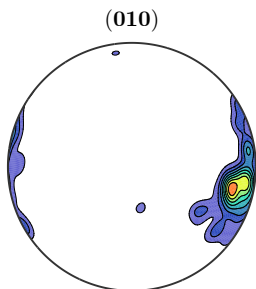
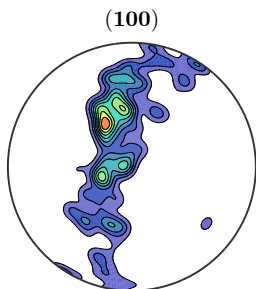
```
plotPDF(O, h, 'contourf')
```

specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

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

```
plotIPDF(O, v, 'contourf')
```



Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

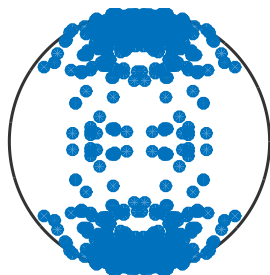
```
plotPDF(O, h, 'contourf')
```

specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

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

```
plotIPDF(O, v, 'contourf')
```



Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

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

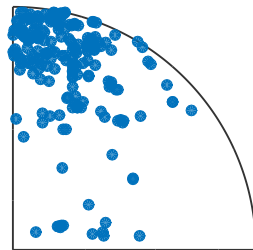
specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

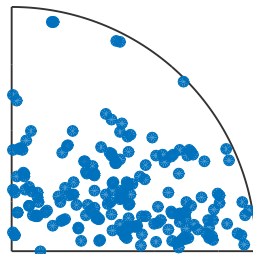
```
v = [vector3d.X, vector3d.Y]
plotIPDF(O, v)
```

```
plotIPDF(O, v, 'contourf')
```

100



010



Pole Figures and Inverse Pole Figures

Lattice planes in specimen coordinates

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

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

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

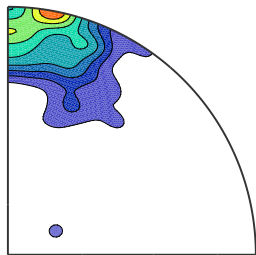
specimen directions in crystal coordinates

```
plot(symmetrise(inv(O)) * vector3d.X)
plot(symmetrise(inv(O)) * vector3d.Y)
```

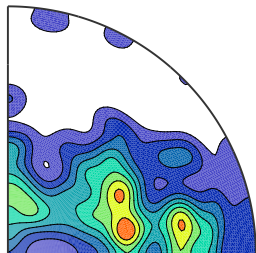
```
v = [vector3d.X, vector3d.Y]
plotIPDF(O, v)
```

```
plotIPDF(O, v, 'contourf')
```

100

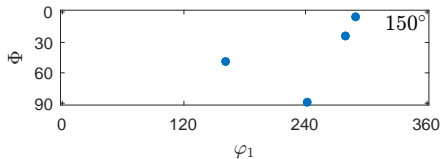
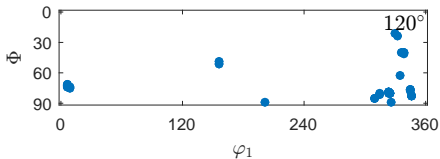
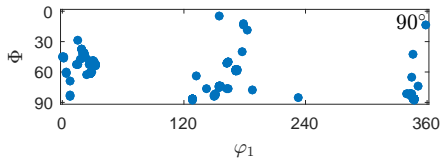
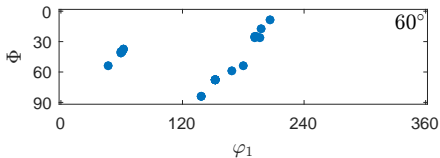
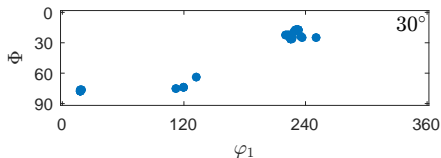
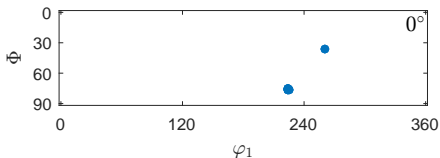


010



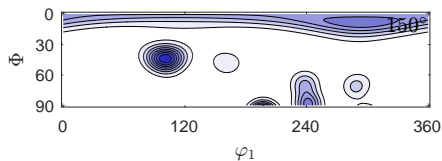
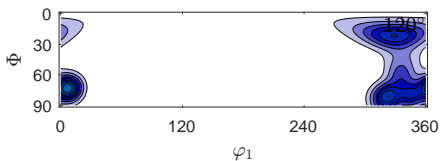
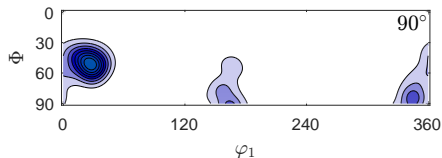
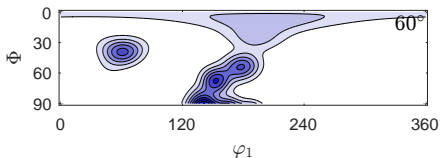
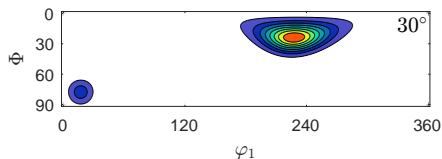
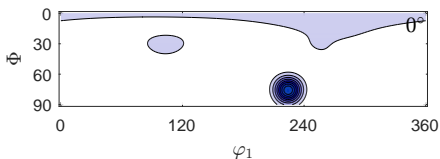
Plotting in Orientation Space

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



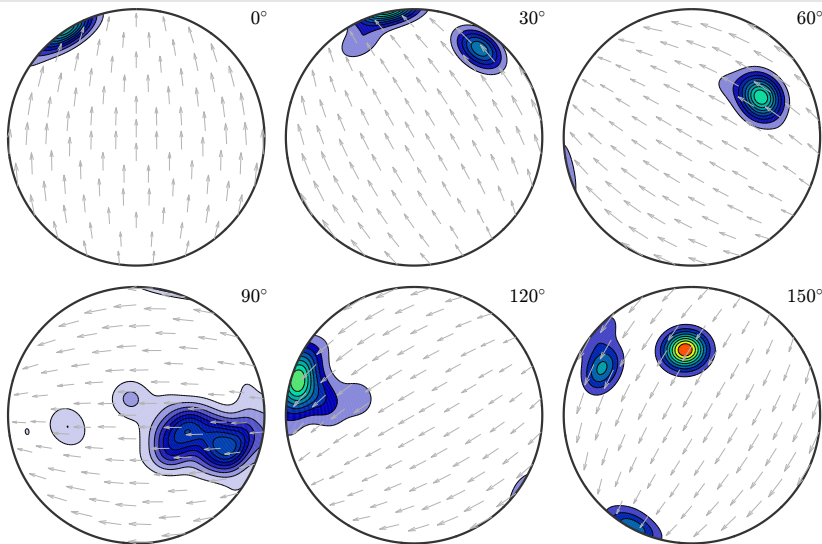
Plotting in Orientation Space

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



Plotting in Orientation Space

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



Plotting in Orientation Space

```
plotSection(0, 'AxisAngle', (10:15:115)*degree, ...
            'contourf')
```

$\omega = 10^\circ$



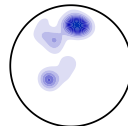
$\omega = 25^\circ$



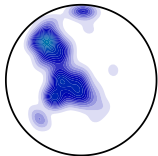
$\omega = 40^\circ$



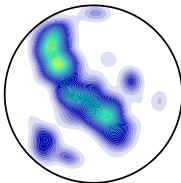
$\omega = 55^\circ$



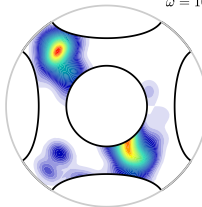
$\omega = 70^\circ$



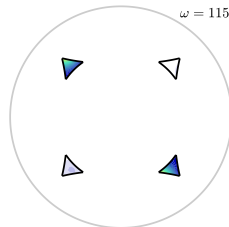
$\omega = 85^\circ$



$\omega = 100^\circ$



$\omega = 115^\circ$



The Orientation Space

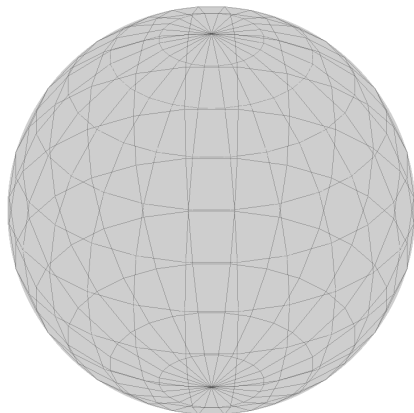
plot(orientationRegion)

```
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

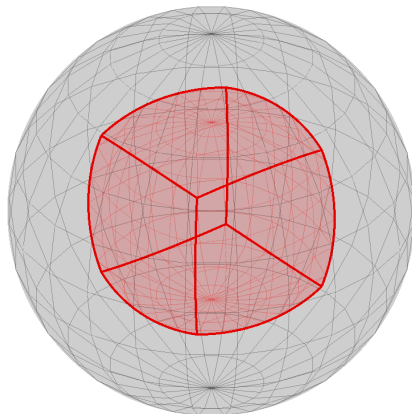
```
plot(orientationRegion)
```

```
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

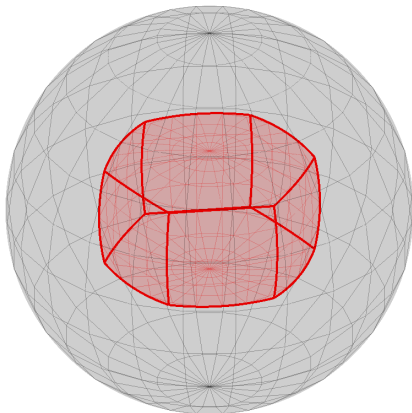
```
plot(orientationRegion)
```

```
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
```



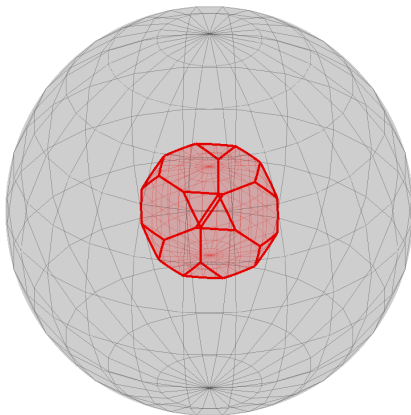
The Orientation Space

```
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

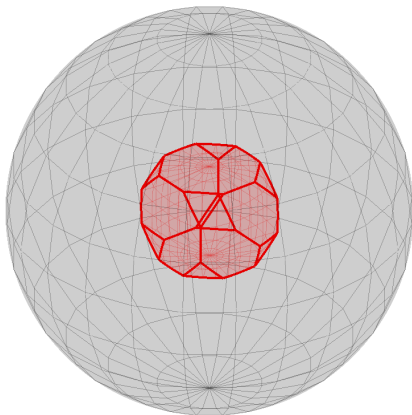
```
plot(orientationRegion)
```

```
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 = 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

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

volume portions

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

export to ASCII file

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

export to ASCII file

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

Operations on Orientations

mean orientation

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

mean orientation spread

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

volume portions

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

export to ASCII file

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

Operations on Orientations

mean orientation

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

mean orientation spread

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

volume portions

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

export to ASCII file

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

Fibres

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

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

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

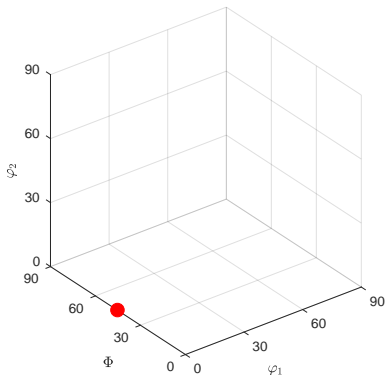
```
f.symmetrise
```

```
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

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

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

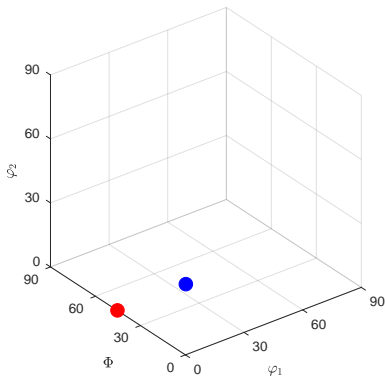
f.symmetrise

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

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

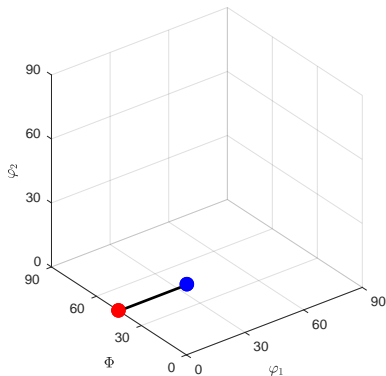
```
f = fibre( o1 , o2 )
```

```
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)
```

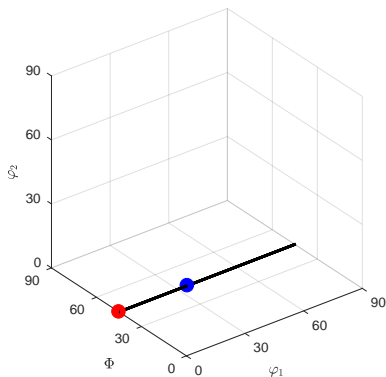
```
f = fibre(o1, o2, 'full')
```

```
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
```

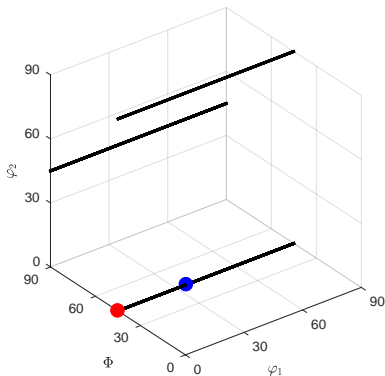
```
symmetry: 222
```

```
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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```

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f.symmetrise
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f = fibre.beta( cs , ss )
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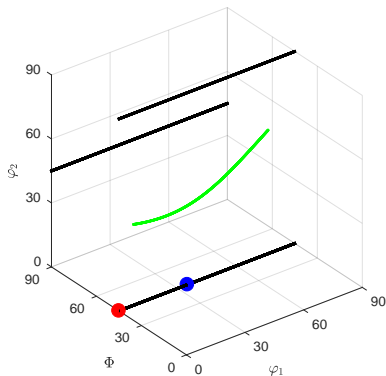
```
h = Miller( 1 , 1 , 1 , cs )
```

```
f = fibre( h , vector3d.Z )
```

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

```
angle( ori , f )
```

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



Fibres

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```

```
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```

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

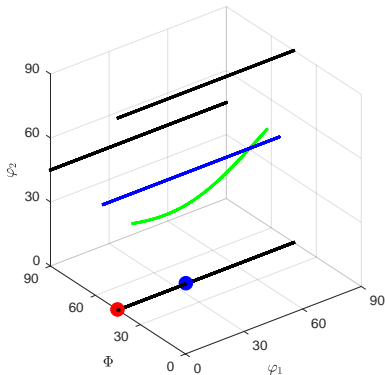
```
h = Miller( 1 , 1 , 1 , cs )
```

```
f = fibre( h , vector3d.Z )
```

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

```
angle( ori , f )
```

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

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

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```

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

```
f.symmetrise
```

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

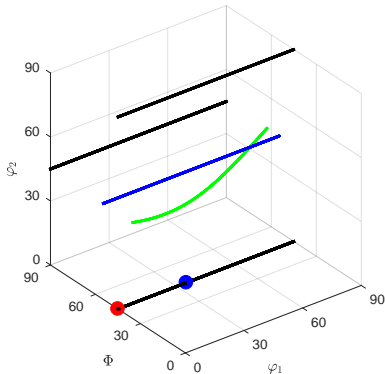
```
h = Miller( 1 , 1 , 1 , cs )
```

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

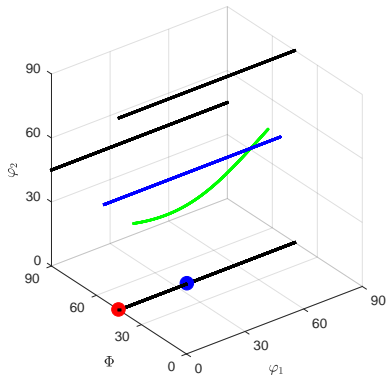
f.symmetrise

f = fibre.beta( cs , ss )

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

f = fibre.fit( ori )

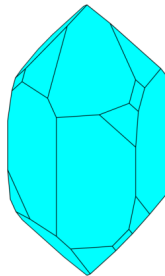
angle( ori , f )
volume( ori , f , 5 * degree )
```



Simple Crystal Shapes

```
cS = crystalShape . quartz
```

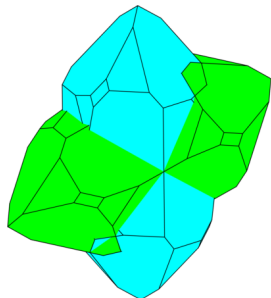
```
cS = crystalShape (show methods, plot)  
mineral: Quartz (321, X||a*,Y||b,Z||c*)  
vertices: 56  
faces: 30
```



Simple Crystal Shapes

```
cS = crystalShape . quartz
```

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

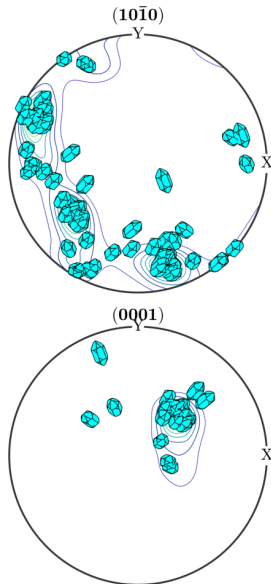


Simple Crystal Shapes

```
cS = crystalShape.quartz
```

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

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



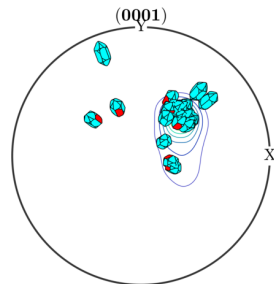
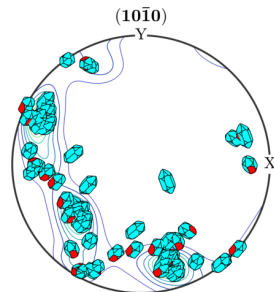
Simple Crystal Shapes

```
cS = crystalShape . quartz
```

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

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

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



Vectors

○○○○○○○○

Rotations

○○○○○

Crystal Symmetries

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Miller Indices

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Orientations

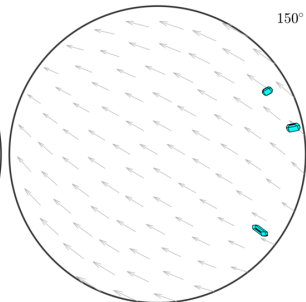
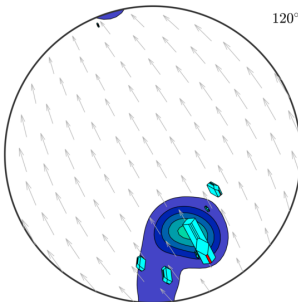
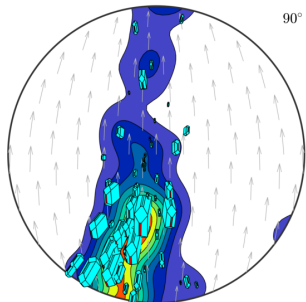
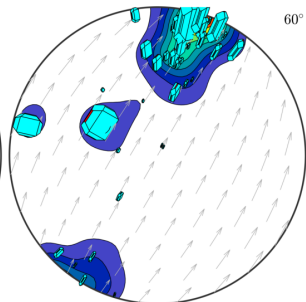
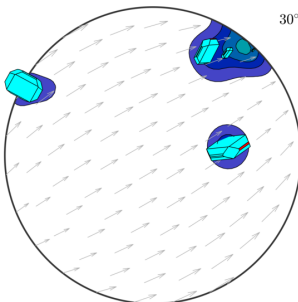
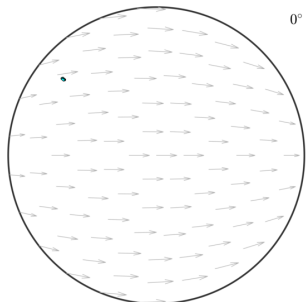
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Fibres

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Crystal Shapes

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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')
```