Crystal Geometry

MTEX - A Texture Calculation Toolbox

R. Hielscher

Faculty of Mathematics,
Chemnitz University of Technology, Germany

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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)
```

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

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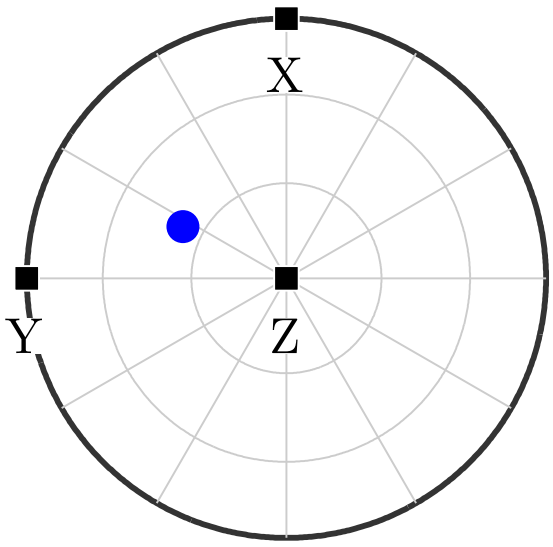
```
plotx2north, plotzOutOfPlane
plot(r)
```



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

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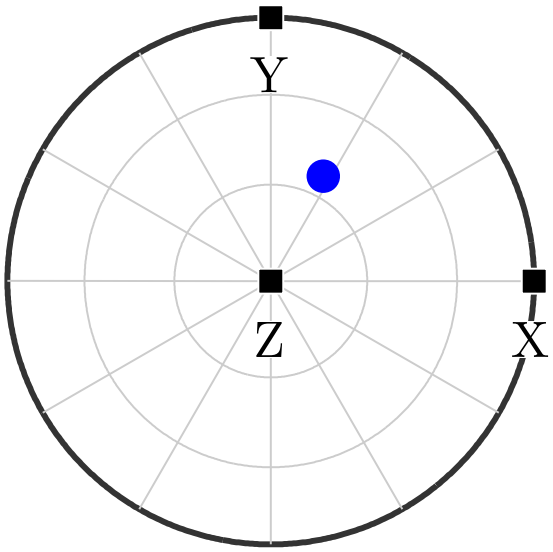
```
plotx2east, plotzOutOfPlane
plot(r)
```



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Defining vectors

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

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

predefined vectors

```
r = xvector, r = yvector, r = zvector
```

combine vectors

```
r = [xvector, yvector, vector3d(1,1,1)];
```

importing vectors

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

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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
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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*xvector - yvector;
```

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.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

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single out vectors by a logical condition

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

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

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  x y z
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  1 1 0
```

single out vectors by a logical condition

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The above techniques applies also to pole figure data, orientations, EBSD data, grains, 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) = yvector
```

remove the second vector completely

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

change the x coordinate of all vectors

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```
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  x y z
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  0 1 0
  1 1 1
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remove the second vector completely

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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
```

Changing Vectors

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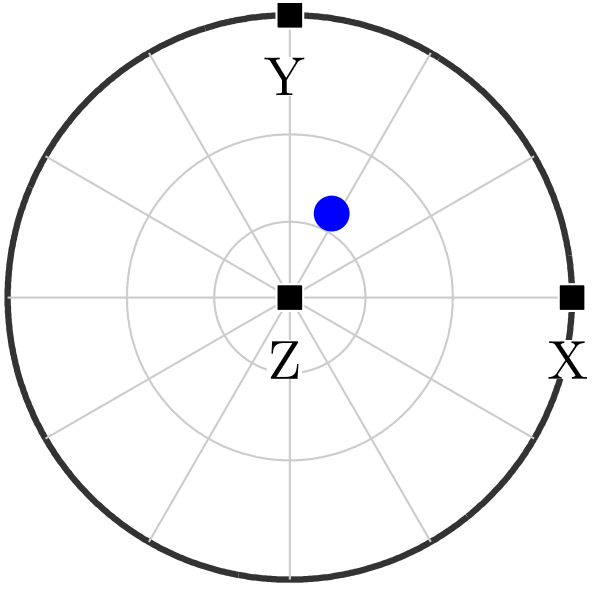
The above techniques applies also to pole figure data, orientations, EBSD data, grains, etc.

Plotting Vectors

spherical projections: `earea`, `edist`, `eangle`
hemisphere: `upper`, `lower`

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



combined plots

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

plot color coded data

```
r = randv(100)  % 100 random points
plot(r,1:100)
% colored by their number
```

Plotting Vectors

spherical projections: `earea`, `edist`, `eangle`
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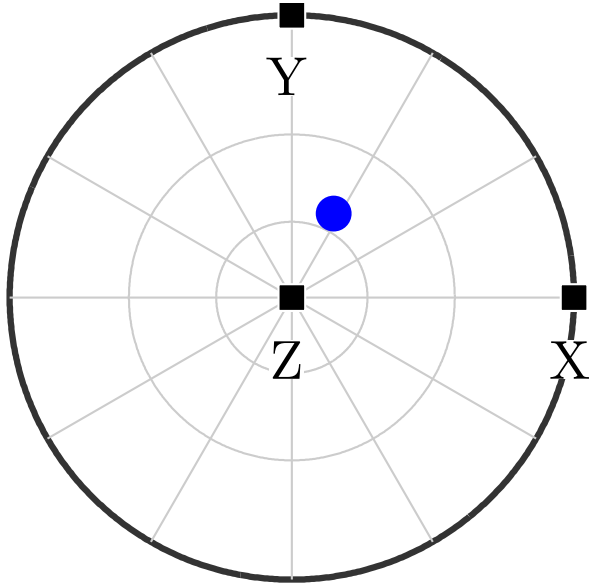
plot(r,'projection','earea','upper')
```



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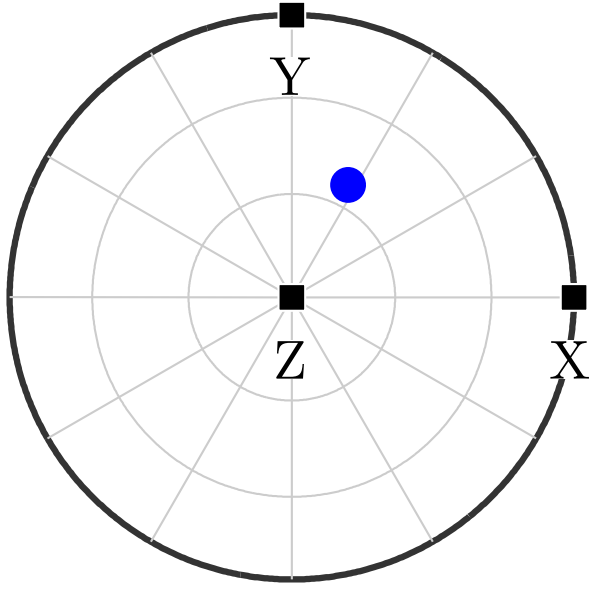

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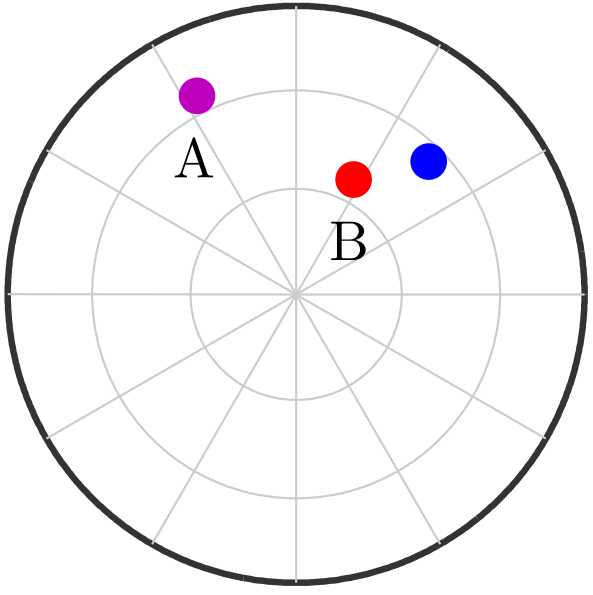

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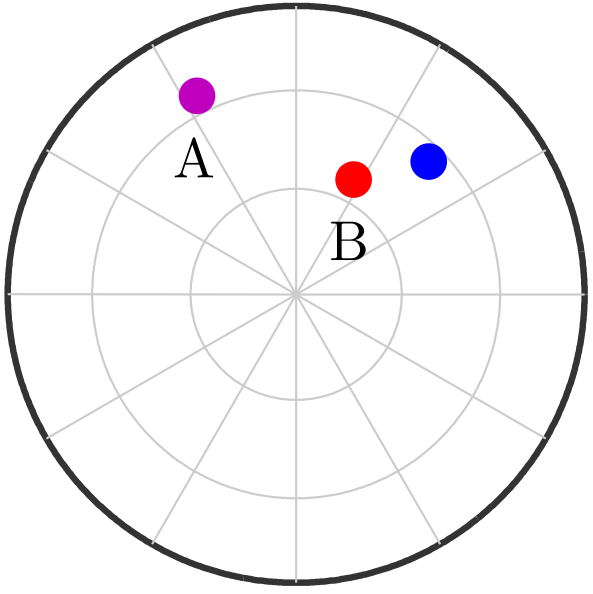

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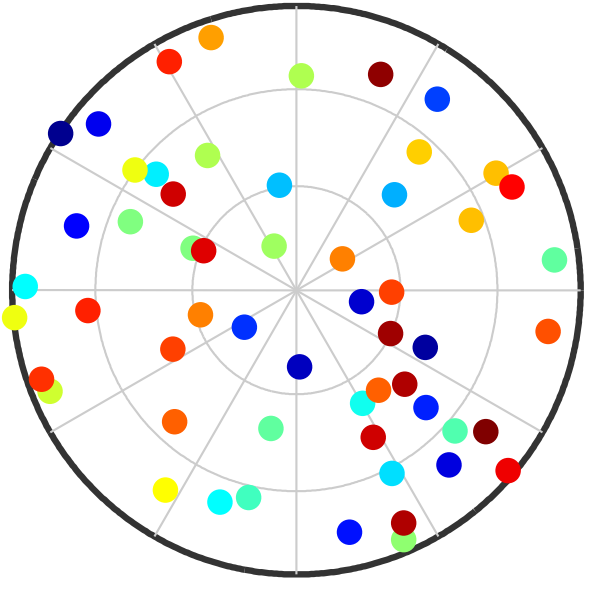


Customize Plots

General Syntax

```
annotate(vector3d,<options>)
```

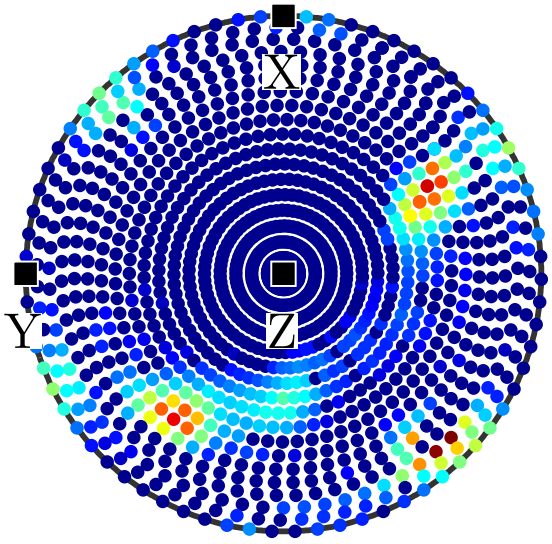
Options

```
Marker                % marker shape
MarkerSize            % marker size
MarkerFaceColor       % face color
MarkerEdgeColor       % edge color
label                 % a label text
color, background     % text colors
```

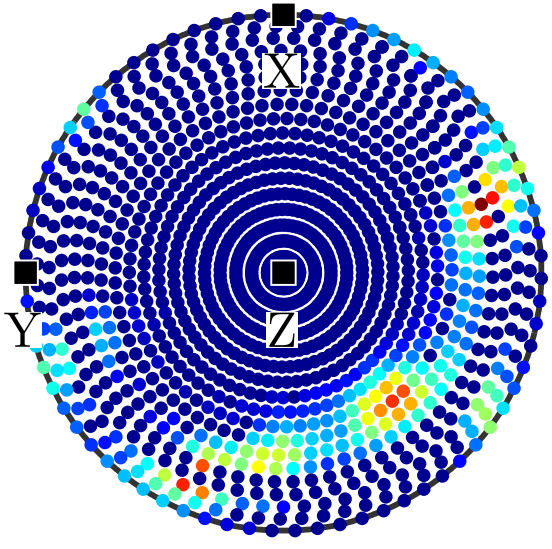
Example

```
annotate([xvector,yvector,zvector],
  'Backgroundcolor','w','Marker','s',
  'MarkerEdgeColor','w','labeled',
  'MarkerFaceColor','k')
```

(02–21)



(10–10)



Customize Plots

General Syntax

```
annotate(orientation,<options>)
```

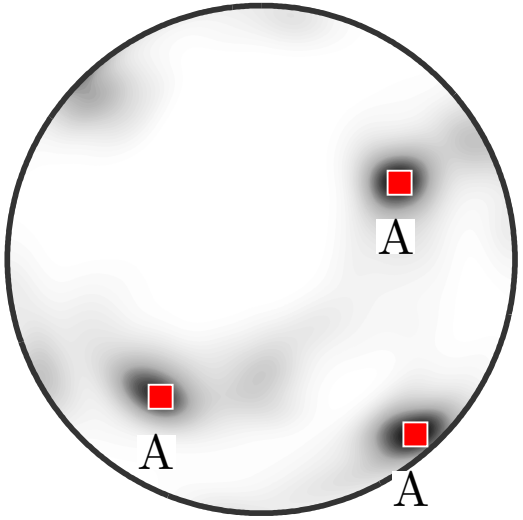
Options

```
Marker                % marker shape
MarkerSize            % marker size
MarkerFaceColor       % face color
MarkerEdgeColor       % edge color
label                 % a label text
color, background     % text colors
```

Example

```
annotate(q0,'label','A',...
  'Backgroundcolor','w','Marker','s',
  'MarkerEdgeColor','w',...
  'MarkerFaceColor','r')
```

(02–21)



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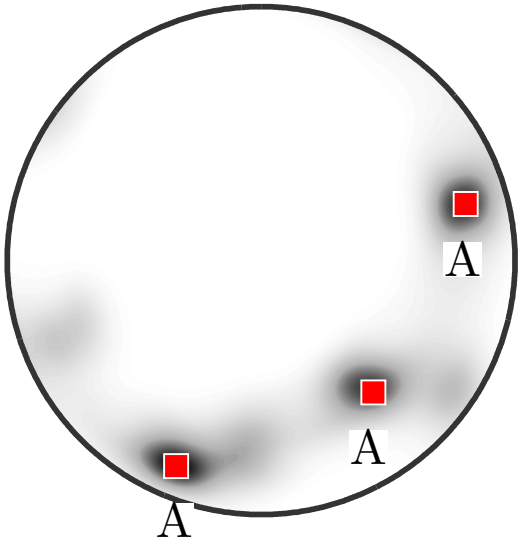


Axes

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

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

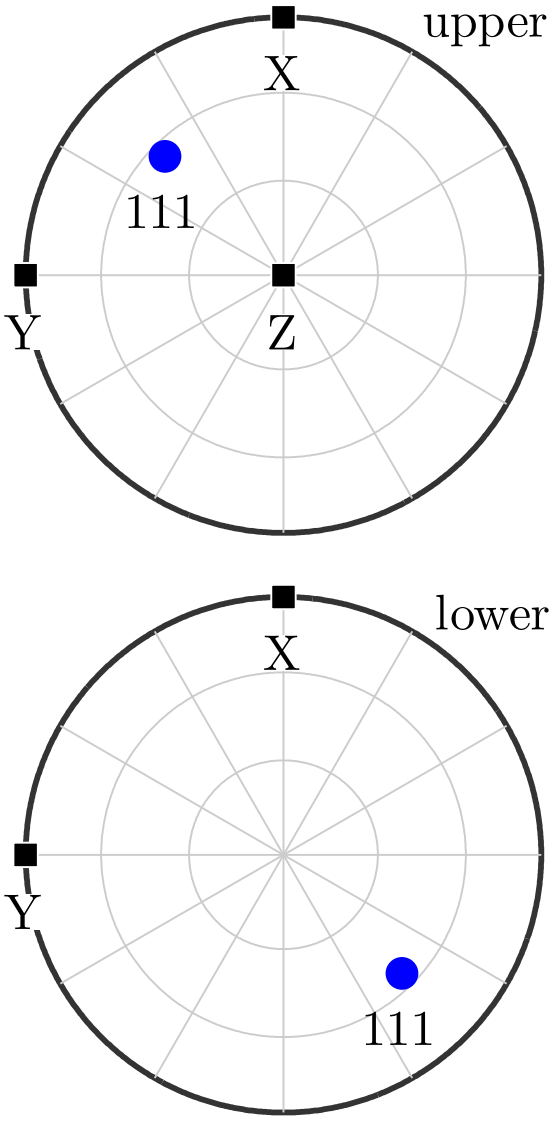
Then `r` and `-r` represent the same axis

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

The angle to an axis is always less then 90°

```
angle(r,-xvector) / degree
```

The option **antipodal** in a contour plot



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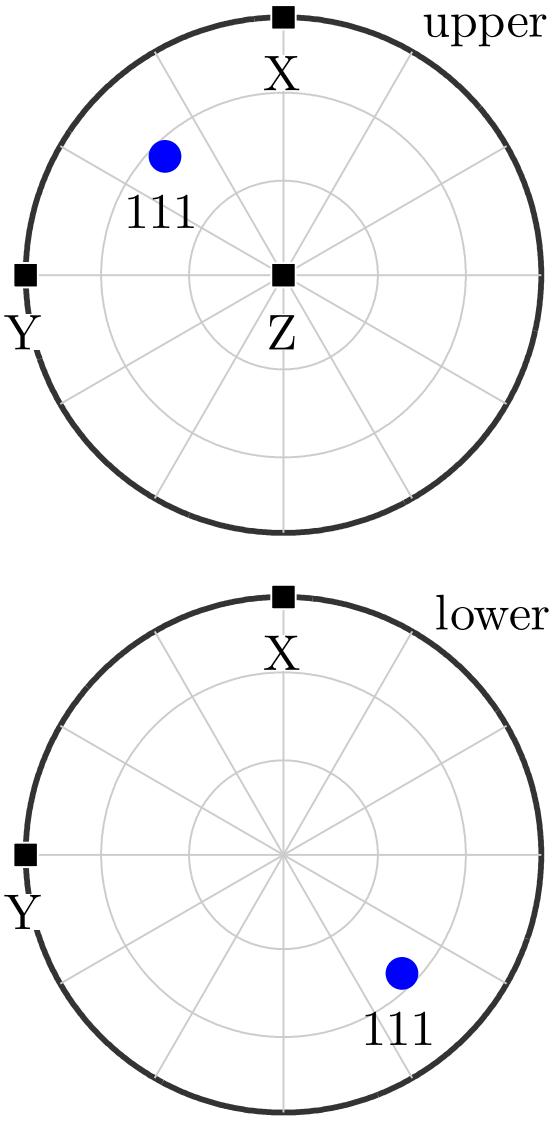

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```
  54.7
```

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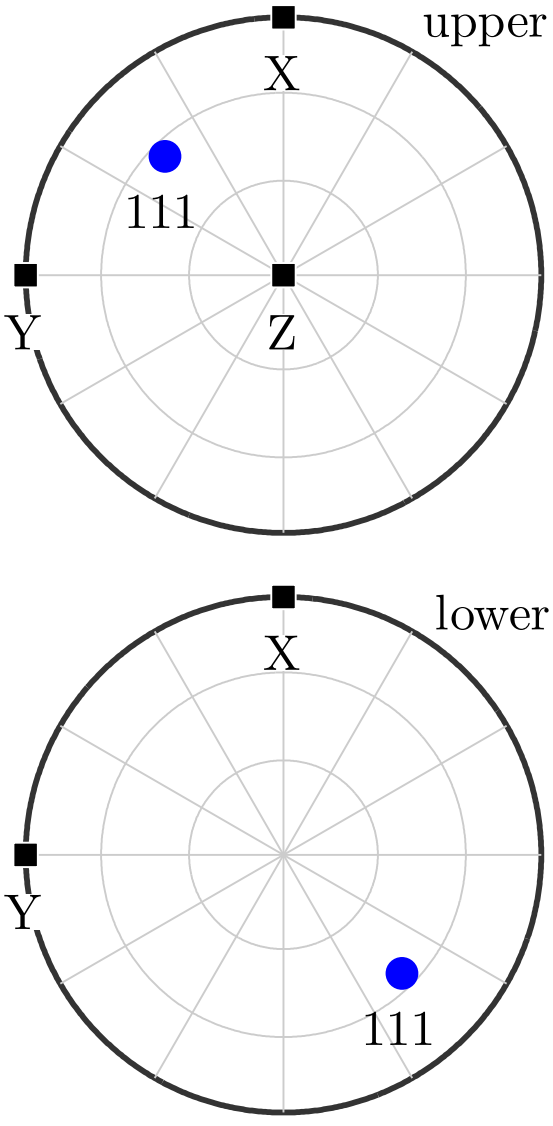

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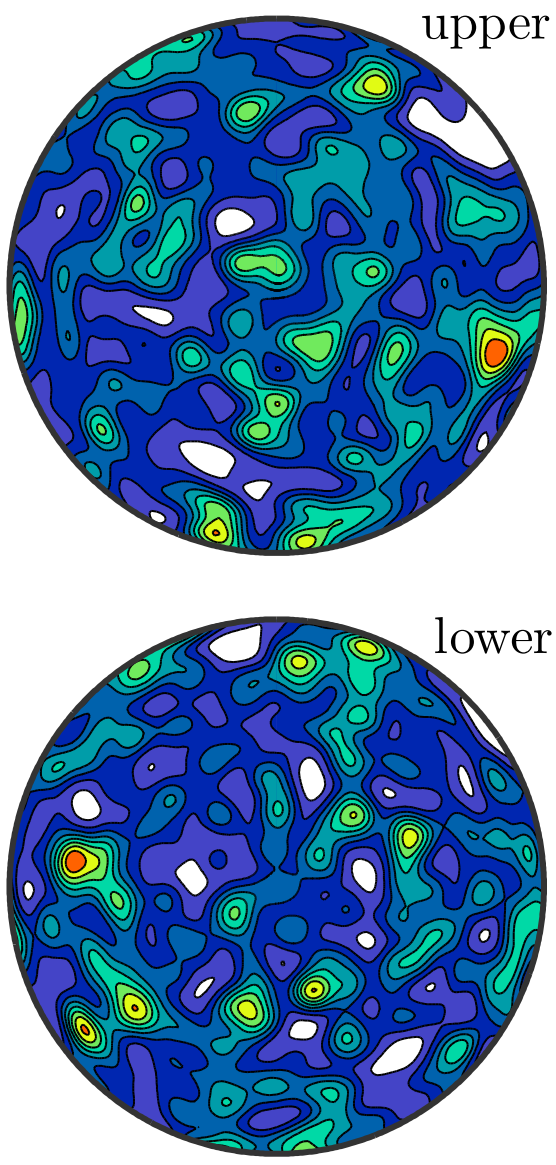
```
r = randv(1000)
plot(r,'contourf')
```



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plot(r,'contourf','antipodal')
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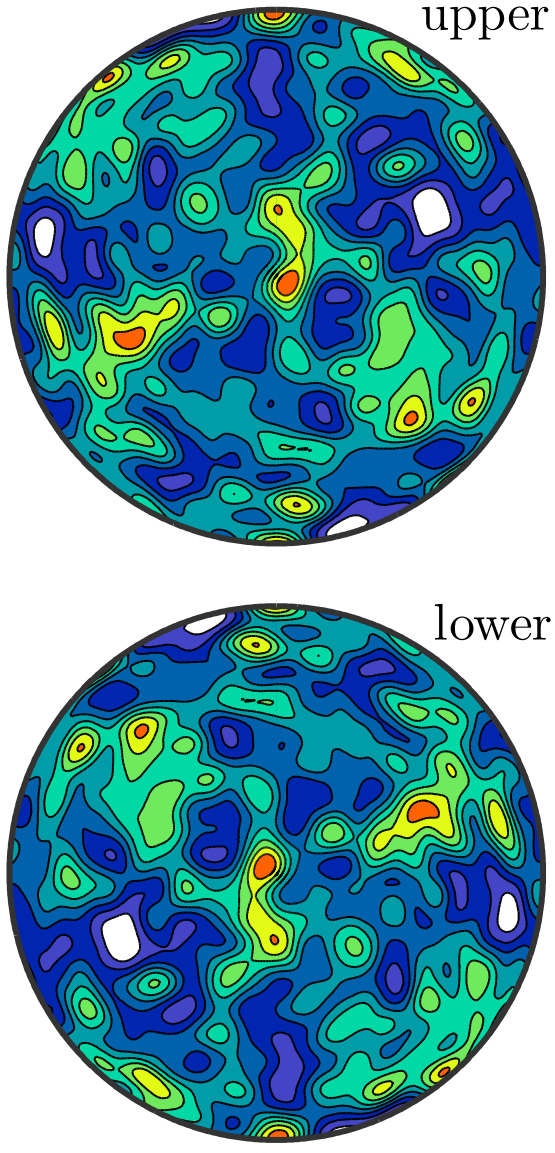

Rotations

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

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

Most commonly, rotations are given by Bunge Euler angles.

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

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

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

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
   100    20   300     0
```

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

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```

```
R = rotation (show methods, plot)
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  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',xvector,'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 **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

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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',xvector,...
             '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

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

combine rotations

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     0    0    0    0
```

Basic Calculations

rotate a vector

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R = rotation('axis',xvector,...
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R * vector3d(0,1,1)
```

the inverse rotation

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```

combine rotations

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

plotting

```
scatter(R) % Rodriguez space
```

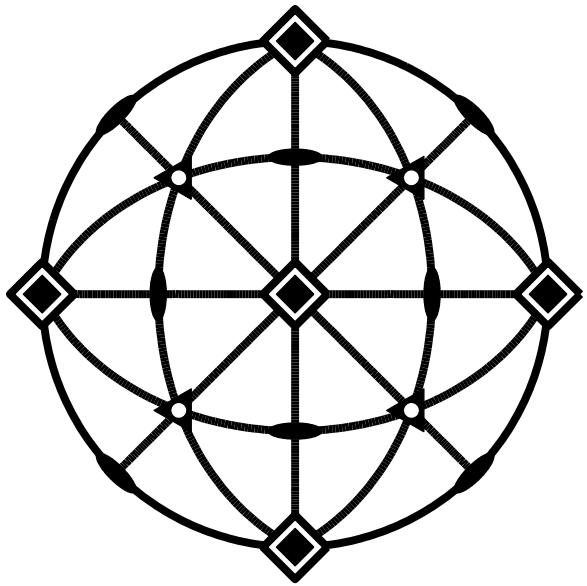
Crystal Symmetry

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

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

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

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

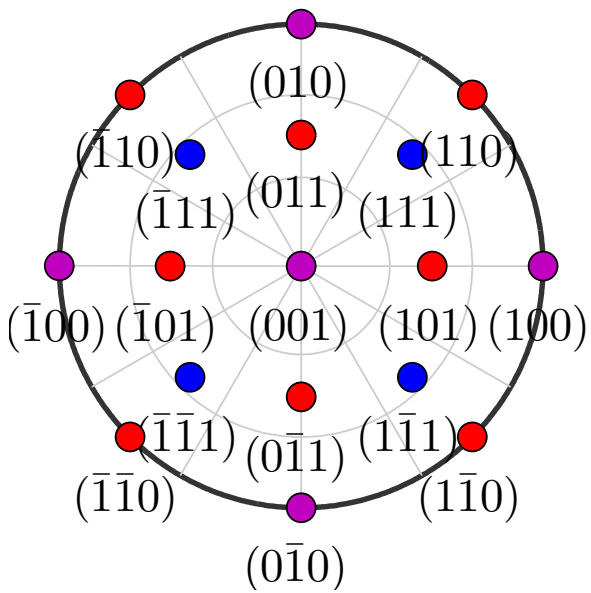


extract the rotations of a point group

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

import data from crystal information files

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



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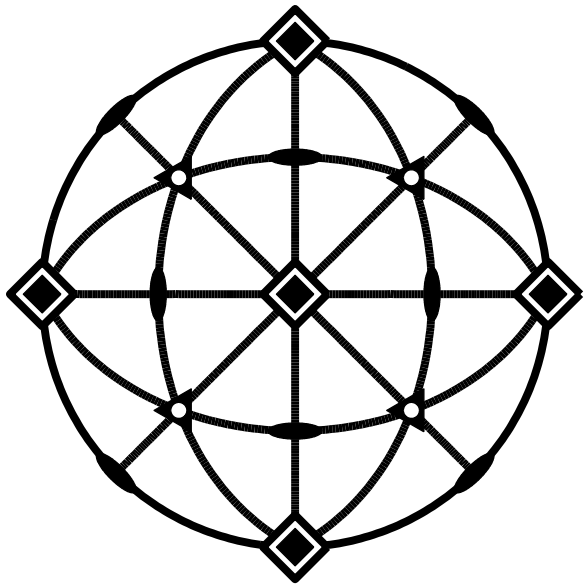
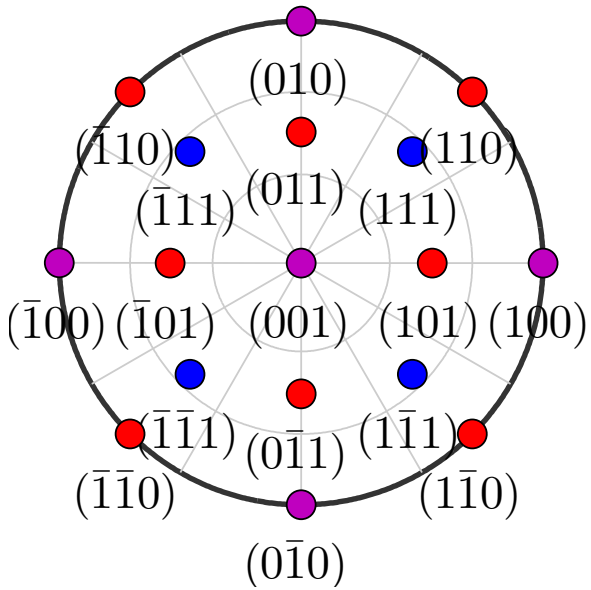


extract the rotations of a point group

```
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
```



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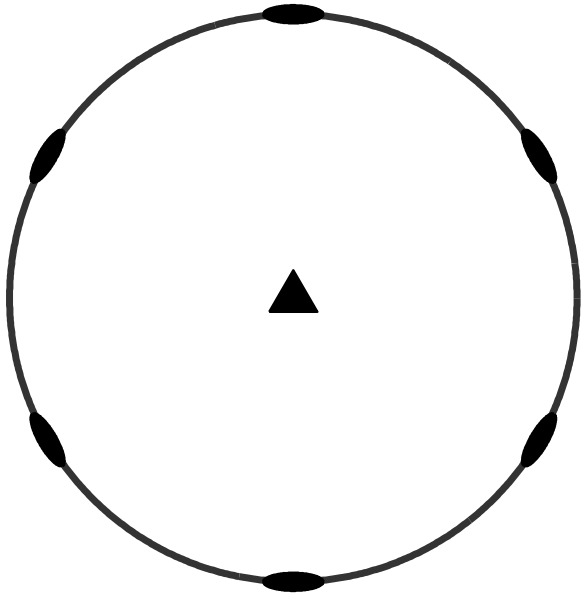

extract the rotations of a point group

```
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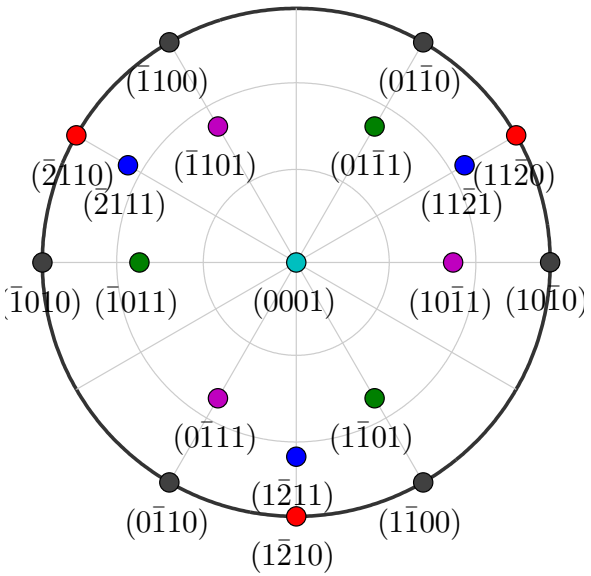
import data from crystal information files

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

```
C = 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*
```



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])
```

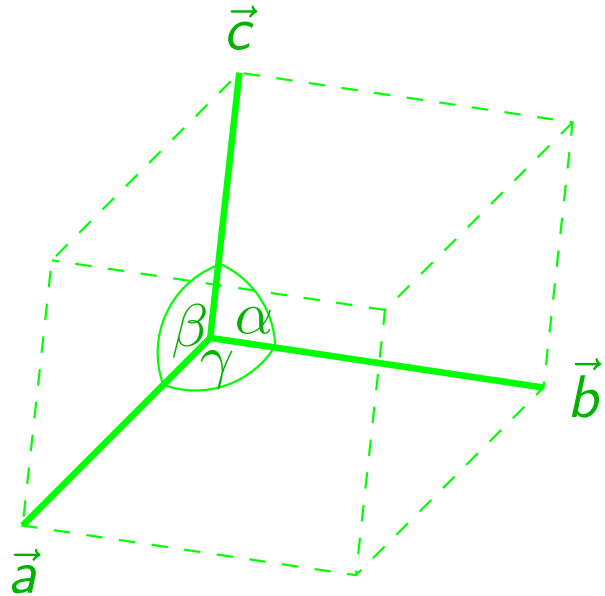
The axes of the reciprocal lattice are defined orthogonal to $\vec{a}, \vec{b}, \vec{c}$, i.e.

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

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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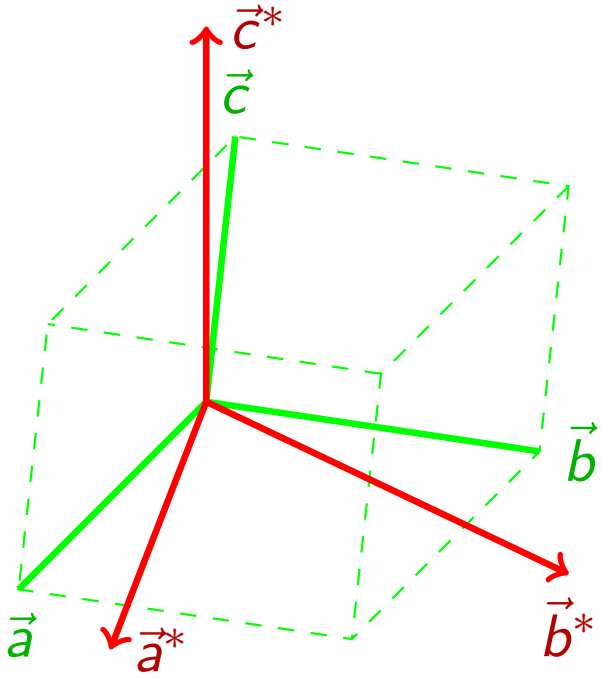

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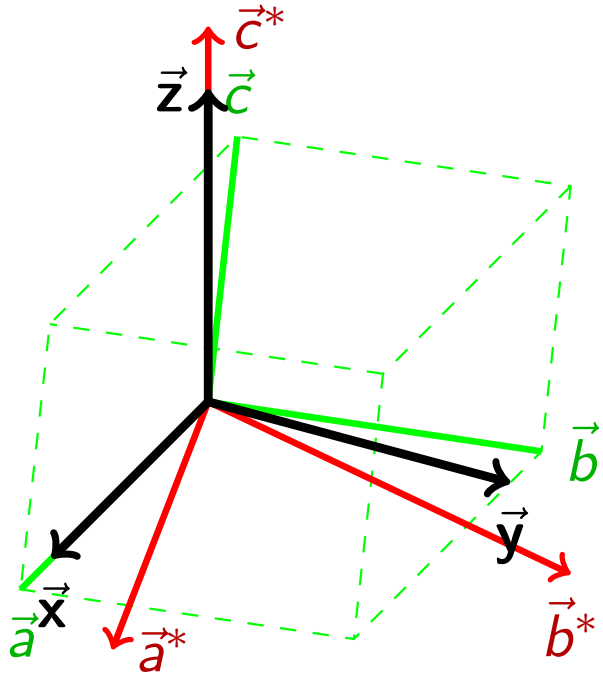


```
C = crystalSymmetry('321',[a b c], 'X||a', 'Z||c*')
```

Unit Cell, Reciprocal and Orthogonal Coordinate System

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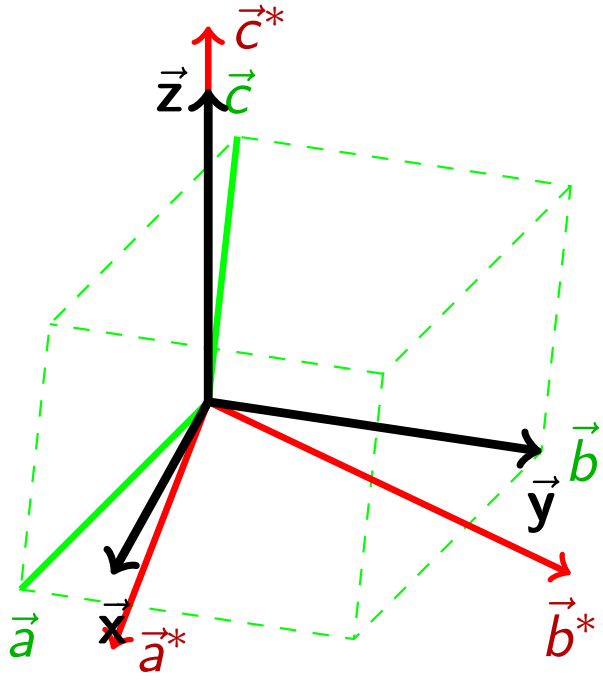


```
C = crystalSymmetry('321',[a b c],'X||b','Z||c*')
```

Miller Indices - Crystal Fixed Directions

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

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

Miller Indices - Crystal Fixed Directions

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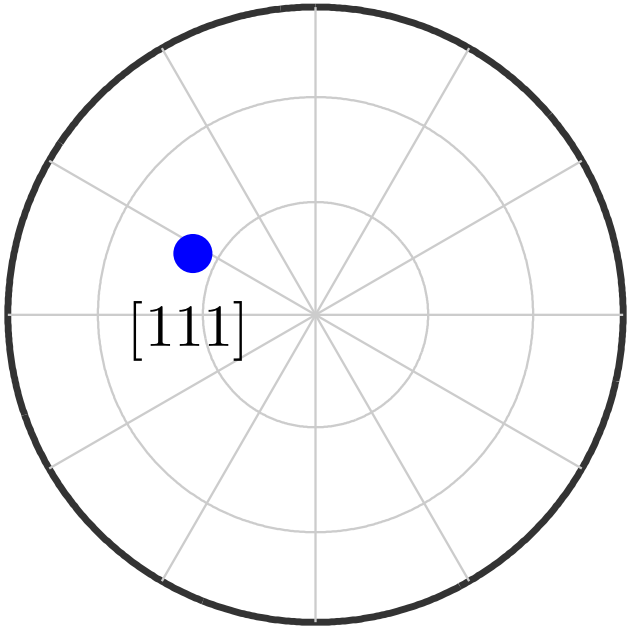
$$\vec{m} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}.$$

```
C = symmetry('mmm',[1 2 3])
m = Miller(1,1,1,C,'uvw')
```

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




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

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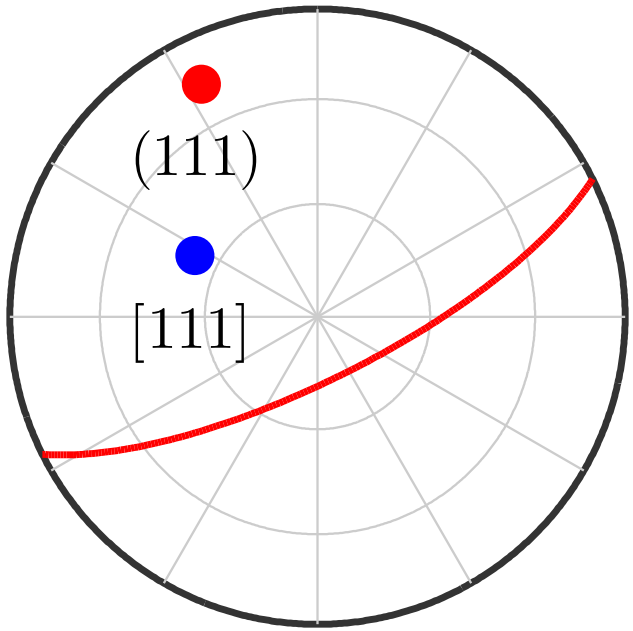

A direction in reciprocal coordinates

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

```
m = Miller(1,1,1,C,'hkl')
```

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

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

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

```
plot(m,'plane')
```

Miller Indices - Crystal Fixed Directions

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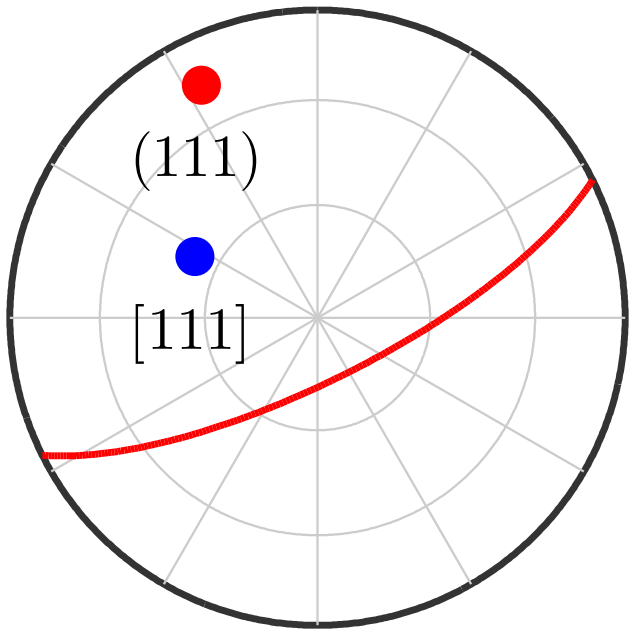
```



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

```
m = Miller(1,1,1,C,'hkl')
```

A direction in the orthogonal coordinate system

```
m = Miller(xvector,S)
```

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

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

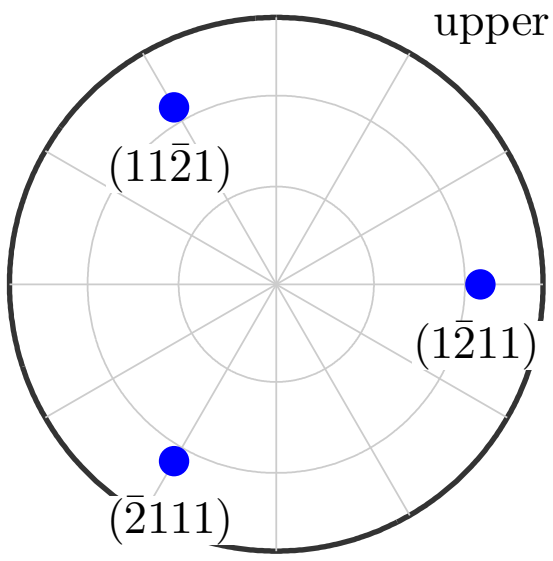
```
plot(m,'plane')
```

Calculating with Crystal Directions

Find all symmetrically equivalent directions

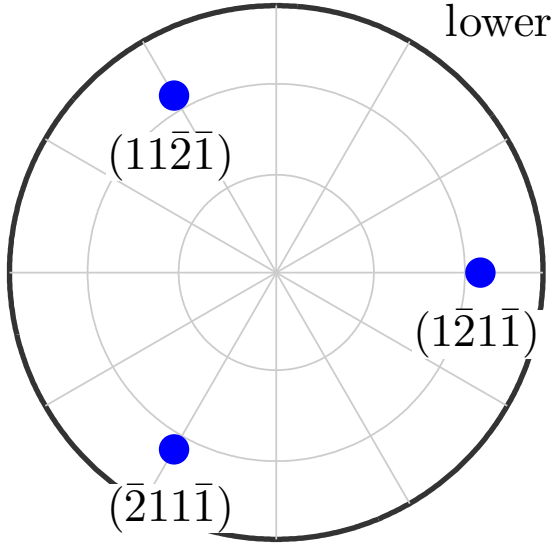
```
C = loadCIF('quartz')
m = Miller(1,1,-2,1,C)
symmetrise(m)
```

```
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
```



Plot all symmetrically equivalent directions

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



Compute angle modulo symmetry

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

Calculating with Crystal Directions

Find all symmetrically equivalent directions

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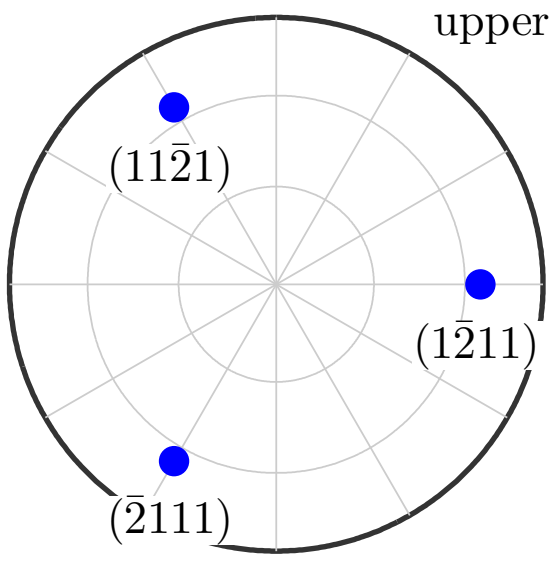
```

Plot all symmetrically equivalent directions

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



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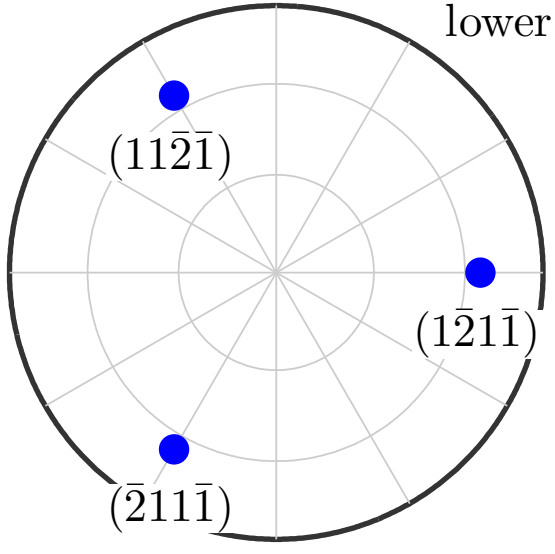

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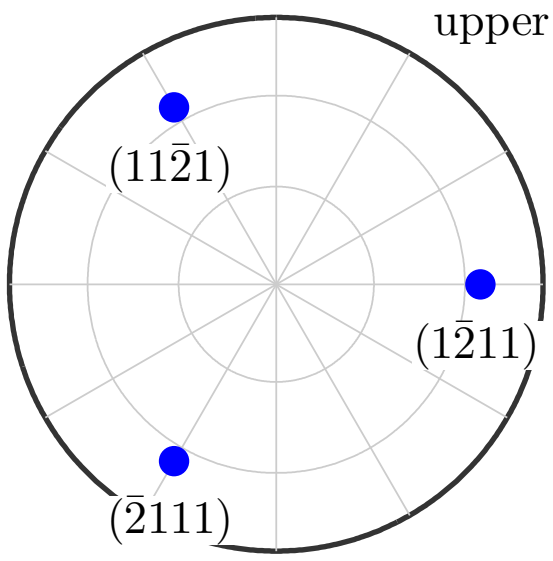

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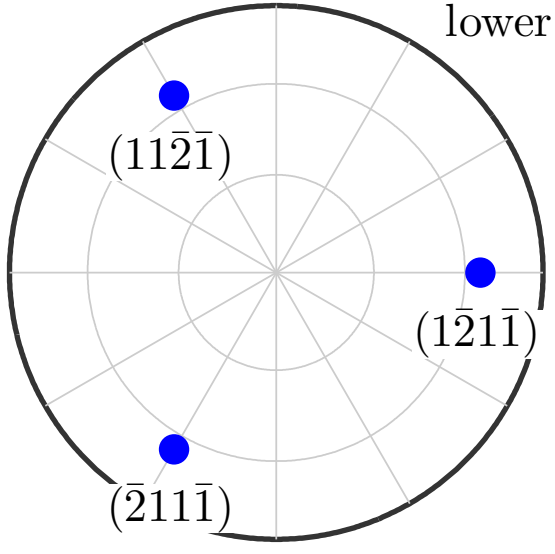


Crystal Orientations

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.,

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

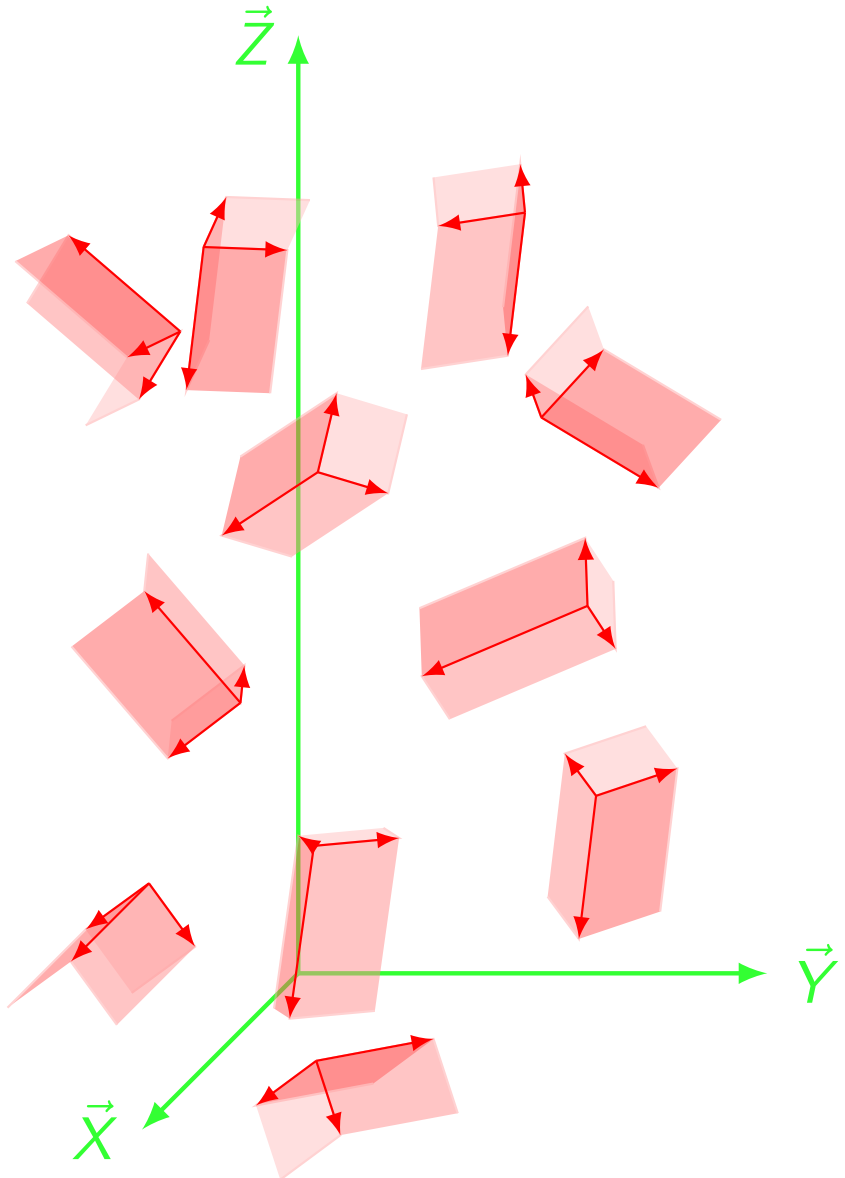
The coordinate transform $\mathbf{O}$ with

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

is called crystal orientation.

The orientation $\mathbf{O}$ maps the specimen coordinate system $\vec{X}, \vec{Y}, \vec{Z}$ onto the crystal coordinate systems $\vec{x}, \vec{y}, \vec{z}$.

The orientation $\mathbf{O}$ is well defined only up the crystal symmetry.



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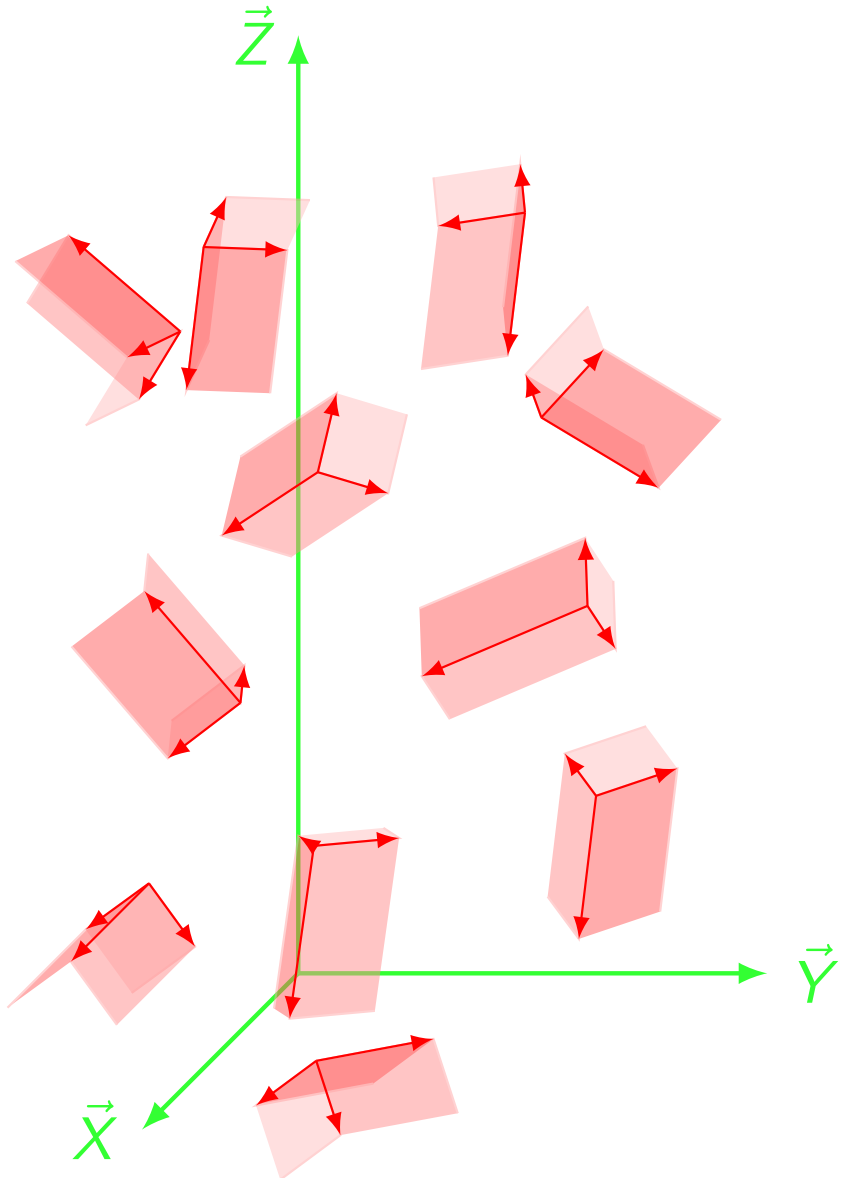

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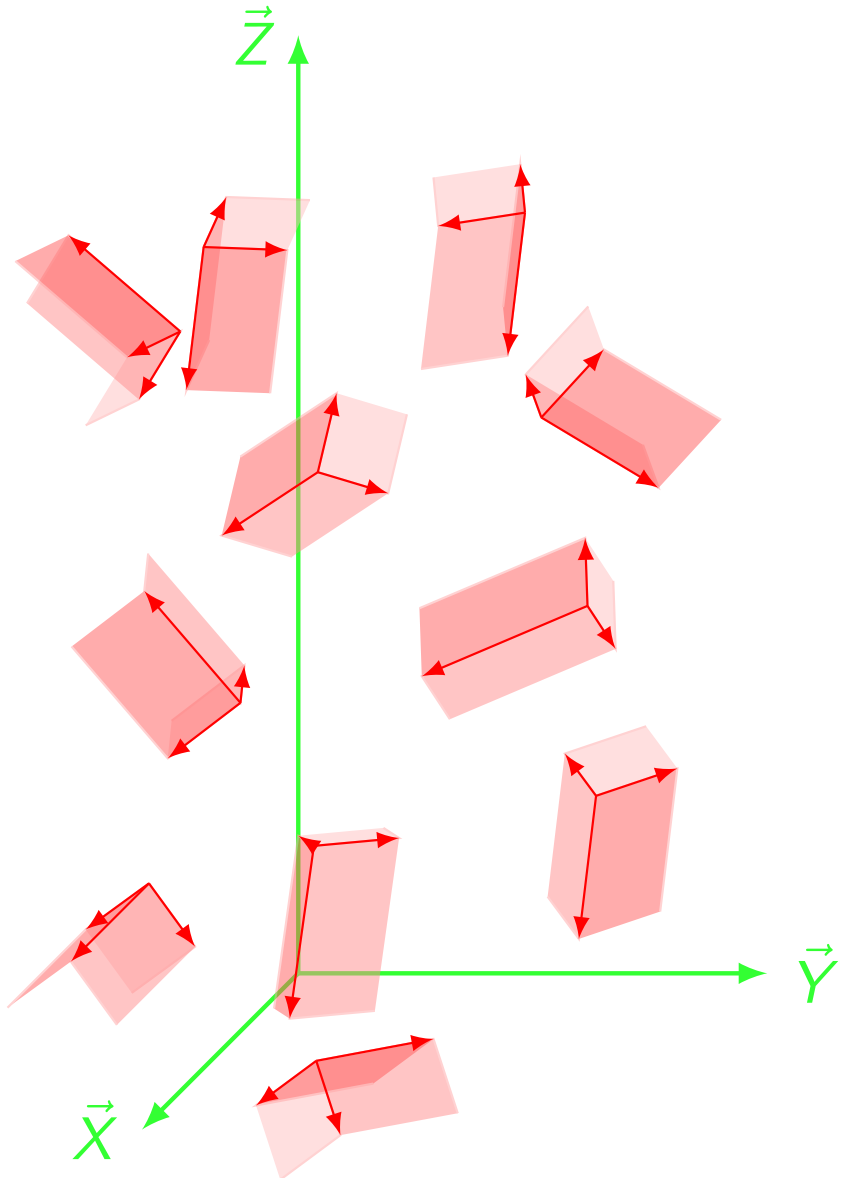


Crystal Orientations

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.,

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

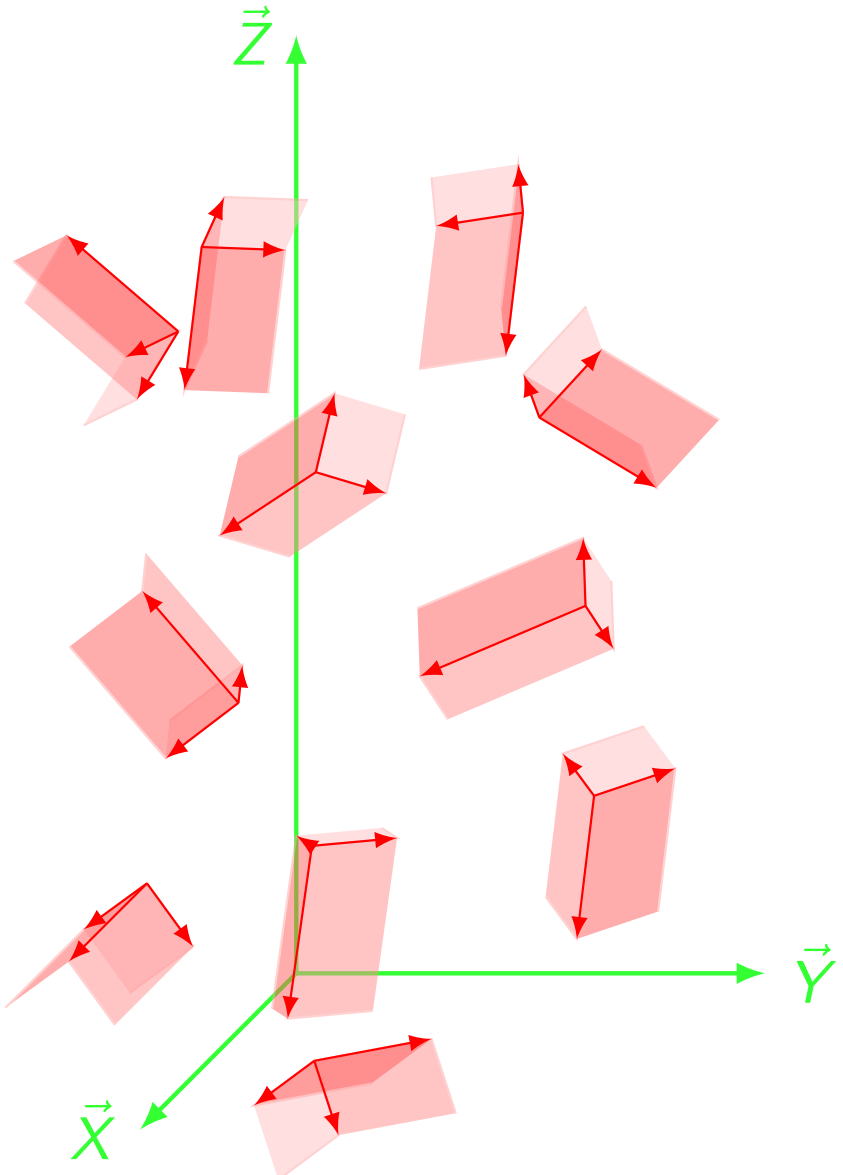
The coordinate transform $\mathbf{O}$ with

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

is called crystal orientation.

The orientation $\mathbf{O}$ maps the specimen coordinate system $\vec{X}, \vec{Y}, \vec{Z}$ onto the crystal coordinate systems $\vec{x}, \vec{y}, \vec{z}$.

The orientation $\mathbf{O}$ is well defined only up the 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

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```

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  = brassOrientation(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  = brassOrientation(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',zvector,'angle',90*degree)
```

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',zvector,'angle',90*degree)
O2 = R * O1
```

Coordinate Transforms

Remember, an orientation converts crystal into specimen coordinates

```
r = O * Miller(1,0,-1,0,CS)
```

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

its inverse converts specimen into crystal coordinates

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

Hence, for two orientation $\mathbf{O_1}$ and $\mathbf{O_2}$ the concatenation $\mathbf{inv(O_2)O_1}$ converts crystal coordinates into crystal coordinates

```
O2 = inv(O2) * O1 * Miller(1,0,-1,0,CS)
```

Coordinate Transforms

Remember, an orientation converts crystal into specimen coordinates

```
r = O * Miller(1,0,-1,0,CS)
```

its inverse converts 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
```

Hence, for two orientation $\mathbf{O_1}$ and $\mathbf{O_2}$ the concatenation $\mathbf{inv(O_2)O_1}$ converts crystal coordinates into crystal coordinates

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O2 = inv(O2) * O1 * Miller(1,0,-1,0,CS)
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Coordinate Transforms

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```
O2 = inv(O2) * O1 * Miller(1,0,-1,0,CS)
```

```
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
```

Misorientations

The misorientation **MO** converts crystal coordinates from one crystal into crystal coordinates of another crystal.

```
MO = inv(O1) * O2
```

```
MO = misorientation (show methods, plot)
  size: 1 x 1
  crystal symmetry: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
  crystal symmetry: Fe (m-3m)

  Roe Euler angles in degree
      Psi    Theta      Phi  Inv.
  2.58238 56.6839   73.197     0
```

compute misorientation angle modulo symmetry

```
angle(O1,O2) / degree, angle(MO) / degree
```

compute the misorientation axis (the axis corresponding to the rotation with minimal angle)

```
axis(MO)
```

Misorientations

The misorientation **MO** converts crystal coordinates from one crystal into crystal coordinates of another crystal.

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Misorientations

The misorientation **MO** converts crystal coordinates from one crystal into crystal coordinates of another crystal.

```
MO = inv(O1) * O2
```

compute misorientation angle modulo symmetry

```
angle(O1,O2) / degree, angle(MO) /degree
```

compute the misorientation axis (the axis corresponding to the rotation with minimal angle)

```
axis(MO)
```

```
ans = Miller (show methods, plot)
  size: 1 x 1
  symmetry: C2
  h -2
  k  3
  l  9
```

An advanced problem

Compute the minimal angle between two crystal directions of different grains having different orientation and different phase.

```
CS1 = loadCIF('quartz'), CS2 = loadCIF('olivin')
```

Define two crystal directions

```
h1 = Miller(1,1,-2,0,CS1), h2 = Miller(1,0,0,CS2)
```

Define two crystal orientations

```
o1 = orientation('Euler',0,50*degree,0,CS1);
o2 = orientation('Euler',60*degree,0,0,CS2);
```

An advanced problem

Compute the minimal angle between two crystal directions of different grains having different orientation and different phase.

```
CS1 = loadCIF('quartz'), CS2 = loadCIF('olivin')
```

```
CS1 = crystal symmetry (show methods, plot)
  mineral            : Quartz
  symmetry           : P 32 2 1 (321)
  a, b, c            : 4.9, 4.9, 5.4
  reference frame    : X||a*, Y||b, Z||c*

CS2 = crystal symmetry (show methods, plot)
  mineral : IRON TETRATHIOSILICATE
  symmetry: P n m a (mmm)
  a, b, c : 12, 7.2, 5.8
```

Define two crystal directions

```
h1 = Miller(1,1,-2,0,CS1), h2 = Miller(1,0,0,CS2)
```

Define two crystal orientations

```
o1 = orientation('Euler',0,50*degree,0,CS1);
```

An advanced problem

Compute the minimal angle between two crystal directions of different grains having different orientation and different phase.

```
CS1 = loadCIF('quartz'), CS2 = loadCIF('olivin')
```

Define two crystal directions

```
h1 = Miller(1,1,-2,0,CS1), h2 = Miller(1,0,0,CS2)
```

```
h1 = Miller (show methods, plot)
  mineral: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
  h  1
  k  1
  i -2
  l  0

h2 = Miller (show methods, plot)
  mineral: IRON TETRATHIOSILICATE (P n m a)
  h 1
  k 0
  l 0
```

Define two crystal orientations

An advanced problem

Compute the minimal angle between two crystal directions of different grains having different orientation and different phase.

```
CS1 = loadCIF('quartz'), CS2 = loadCIF('olivin')
```

Define two crystal directions

```
h1 = Miller(1,1,-2,0,CS1), h2 = Miller(1,0,0,CS2)
```

Define two crystal orientations

```
o1 = orientation('Euler',0,50*degree,0,CS1);
o2 = orientation('Euler',60*degree,0,0,CS2);
```

```
o1 = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry: Quartz (P 32 2 1, X||a*, Y||b, Z||c*)
  sample symmetry : triclinic

  Bunge Euler angles in degree
  phi1  Phi phi2 Inv.
     0   50    0    0
```

The Solution

Compute the coordinates of all there symmetrically equivalent normals with respect to the specimen coordinate system

```
r1 = o1 * symmetrise(h1), r2 = o2 * symmetrise(h2)
```

```
r1 = vector3d (show methods, plot)
  size: 1 x 3
           x           y           z
    0.866025    0.321394    0.383022
   -0.866025    0.321394    0.383022
           0   -0.642788   -0.766044

r2 = vector3d (show methods, plot)
  size: 1 x 2
      x           y           z
    0.5    0.866025           0
   -0.5   -0.866025           0
```

Compute the angles between all combinations of these vectors

```
angles = angle_outer(r1, r2)
```

Compute the minimum of all these angles and convert to degree

The Solution

Compute the coordinates of all there symmetrically equivalent normals with respect to the specimen coordinate system

```
r1 = o1 * symmetrise(h1), r2 = o2 * symmetrise(h2)
```

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angles = angle_outer(r1,r2)
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```
angles =
    0.7794    2.3622
    1.7261    1.4155
    2.1612    0.9804
```

Compute the minimum of all these angles and convert to degree

```
min(angles(:)) ./ degree
```

The Solution

Compute the coordinates of all there symmetrically equivalent normals with respect to the specimen coordinate system

```
r1 = o1 * symmetrise(h1), r2 = o2 * symmetrise(h2)
```

Compute the angles between all combinations of these vectors

```
angles = angle_outer(r1,r2)
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```
angles =
    0.7794    2.3622
    1.7261    1.4155
    2.1612    0.9804
```

Compute the minimum of all these angles and convert to degree

```
min(angles(:)) ./ degree
```

```
ans =
   44.6553
```

Exercise 1

Consider trigonal crystal symmetry.

a) Find all crystallographic directions symmetrically equivalent to $h = (1, 0, \bar{1}, 0)$ (Miller indices)!

b) Find crystallographic directions such that the number of their crystallographic equivalent directions on the upper hemisphere (without equator) is 1, 3, and 6, when including antipodal symmetry!

c) Consider the orientation given by the Euler angles $(30°, 90°, 90°)$ in Bunge convention. Give the Euler angles of all symmetrically equivalent orientations!

d) Which positions in the (0,0,0,1) - pole figure corresponds to the above orientation. Which crystal direction is rotated by this orientation to the specimen direction (0,0,1)?

e) Construct an orientation that rotates the crystallographic directions $(0, 0, 0, 1)$ and $(2, \bar{1}, \bar{1}, 0)$ onto the specimen directions $(1, 0, 0)$ and $(0, 1, 0)$, respectively. Describe the rotation by axis and angle.