Lecture 3 - Rotations and Symmetries

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Active vs. Passive Rotations

Active Rotations

An active rotation is a mapping of the Euclidean space onto itself that keeps at least one point and all distances invariant and preserves orientation.

Passive Rotations

A passive rotation is a coordinate transform from one right handed, orthonormal coordinate system into another one.

Improper Rotations

An improper rotation is a rotation that switches between left handed and right handed coordinate systems.

the matrix $\mathbf{M} = \begin{pmatrix} | & | & | \\ \vec{v}_1 & \vec{v}_2 & \vec{v}_3 \\ | & | & | \end{pmatrix}$

rotates

$\vec{e}_1 \mapsto \vec{v}_1,\ \vec{e}_2 \mapsto \vec{v}_2,\ \vec{e}_3 \mapsto \vec{v}_3$

$\mathbf{M}$ transforms coordinates from the reference frame $(\vec{v}_1, \vec{v}_2, \vec{v}_3)$ into the reference frame $(\vec{e}_1, \vec{e}_2, \vec{e}_3)$

$\tilde{\mathbf{M}} = -\mathbf{M}$ additionally mirrors all vectors at the origin

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

```
r = rotation

  Bunge Euler angles in degree
  phi1  Phi  phi2  Inv.
     0   90     0     0
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
r = rotation.byEuler(0,0,pi/2)
```

```
r = rotation

  Bunge Euler angles in degree
  phi1   Phi   phi2   Inv.
    90     0      0     0
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
r = rotation.byEuler(0,0,pi/2)
```

by a rotation matrix

```
M = [1  0  0;  0  0  -1;  0  1  0]
r = rotation.byMatrix(M)
```

```
r = rotation

  Bunge Euler angles in degree
  phi1   Phi   phi2   Inv.
     0    90      0      0
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
r = rotation.byEuler(0,0,pi/2)
```

by a rotation matrix

```
M = [1 0 0; 0 0 -1; 0 1 0]
r = rotation.byMatrix(M)
```

by pairs of vectors

```
u1 = vector3d.Z; v1 = u1
u2 = vector3d.X; v2 = vector3d.Y
r  = rotation.map(u1,v1,u2,v2)
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
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M = [1  0  0;  0  0  -1;  0  1  0]
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by pairs of vectors

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u1 = vector3d.Z;  v1 = u1
u2 = vector3d.X;  v2 = vector3d.Y
r  = rotation.map(u1,v1,u2,v2)
```

```
r  = rotation.fit(u, v)
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
r = rotation.byEuler(0,0,pi/2)
```

by a rotation matrix

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M = [1 0 0; 0 0 -1; 0 1 0]
r = rotation.byMatrix(M)
```

by pairs of vectors

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u1 = vector3d.Z; v1 = u1
u2 = vector3d.X; v2 = vector3d.Y
r  = rotation.map(u1,v1,u2,v2)
```

```
r  = rotation.fit(u, v)
```

import rotations

```
r = rotation.load('file.txt',...
   'ColumnNames',...
   {'phi1','Phi','phi2'})
```

```
r = rotation
  size: 1 x 100
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

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by a rotation matrix

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M = [1 0 0; 0 0 -1; 0 1 0]
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r  = rotation.map(u1,v1,u2,v2)
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```
r  = rotation.fit(u, v)
```

import rotations

```
r = rotation.load('file.txt',...
  'ColumnNames',...
  {'phi1','Phi','phi2'})
```

random rotations

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

```
r = rotation
  size: 1 x 100
```

Defining Active Rotations

by axis angle

```
v = vector3d(1,0,0)
w = 90*degree
r = rotation.byAxisAngle(v,w)
```

by Euler angles

```
r = rotation.byEuler(0,0,pi/2)
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by a rotation matrix

```
M = [1 0 0; 0 0 -1; 0 1 0]
r = rotation.byMatrix(M)
```

by pairs of vectors

```
u1 = vector3d.Z; v1 = u1
u2 = vector3d.X; v2 = vector3d.Y
r  = rotation.map(u1,v1,u2,v2)
```

```
r  = rotation.fit(u, v)
```

import rotations

```
r = rotation.load('file.txt',...
   'ColumnNames',...
   {'phi1','Phi','phi2'})
```

random rotations

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

identity and inversion

```
r = rotation.id
r = rotation.inversion
```

```
r = rotation

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
     0     0     0     0
     0     0     0     1
```

Defining Active Rotations

by axis angle

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r  = rotation.map(u1,v1,u2,v2)
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r  = rotation.fit(u, v)
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import rotations

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r = rotation.load('file.txt',...
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```

random rotations

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

identity and inversion

```
r = rotation.id
r = rotation.inversion
```

a reflextion

```
r = reflection(vector3d.X)
```

```
r = rotation

  Bunge Euler angles in degree
  phi1   Phi  phi2  Inv.
     0   180     0     1
```

Euler Angles

Definition (Euler angles)

Let $\varphi_1, \varphi_2 \in [0, 2\pi]$ and $\Phi \in [0, \pi]$. Then $\varphi_1, \Phi, \varphi_2$ are called the Euler angles of the rotation

$$\mathbf{R}(\varphi_1, \Phi, \varphi_2) = \mathbf{R}_{\vec{Z},\varphi_1} \mathbf{R}_{\vec{X},\Phi} \mathbf{R}_{\vec{Z},\varphi_2}.$$

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

- For every rotation $\mathbf{R}$ there are Euler angles $\varphi_1, \Phi, \varphi_2$ such that $\mathbf{R} = \mathbf{R}(\varphi_1, \Phi, \varphi_2)$.
- For specific rotations R the Euler angles are not unique, e.g.

$$\mathbf{R}_{\vec{z},\omega} = \mathbf{R}(\varphi_1, 0, \omega - \varphi_1)$$

- Euler angles are the most common way to specify and visualize rotations in texture analysis.
- The ambiguity makes visualization with respect to Euler angles hard to interpret.

Operations with Rotations

vector rotation

```
v = rot .* u
```

concatenation

```
rot = rot1 .* rot2
v = rot .* u
v = rot1 * (rot2 * u)
```

inverse of a rotation / misrotation

```
inv(rot1)
inv(rot1) .* rot2
```

basic statistics

```
mean(rot)
mean(rot,'weights',w)
std(rot)

unique(rot)
```

extract Euler angles

```
[phi1,Phi,phi2] = Euler(rot)
```

extract matrix

```
rot.matrix
```

rotation vectors

```
rot.Rodrigues
rot.homochoric
rot.cubochoric
```

axis / angle

```
rot.axis, rot.angle
angle(rot1,rot2)
```

quaternion

```
[a,b,c,d] = double(rot)
quaternion(rot)
```

Visualizing Rotations

Euler angle space

```
rot = rotation.rand
plot(rot)
```

axis angle space

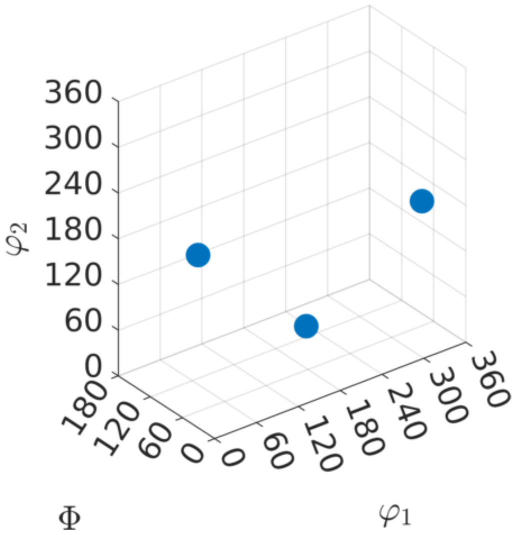
```
plot(rot,'axisAngle')
```

Euler angle φ_2 sections

```
plotSection(rot,'phi2')
```

axis angle sections

```
plotSection(rot,'axisAngle')
```



Visualizing Rotations

Euler angle space

```
rot = rotation.rand
plot(rot)
```

axis angle space

```
plot(rot, 'axisAngle')
```

Euler angle φ_2 sections

```
plotSection(rot, 'phi2')
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axis angle sections

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plotSection(rot, 'axisAngle')
```

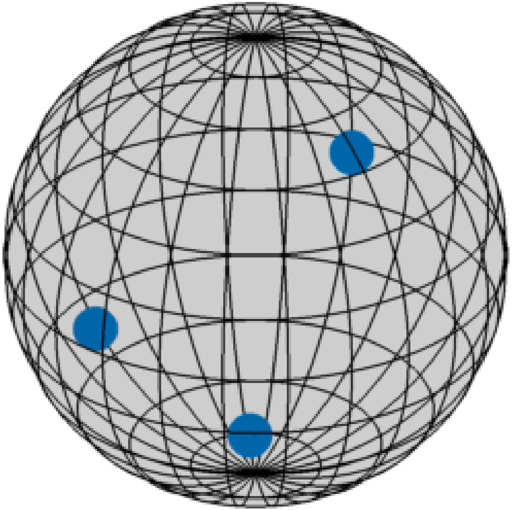

Visualizing Rotations

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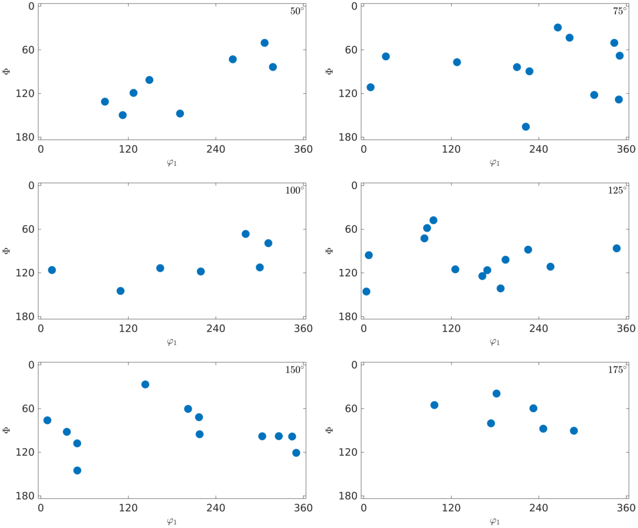

Visualizing Rotations

Euler angle space

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axis angle space

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Euler angle φ_2 sections

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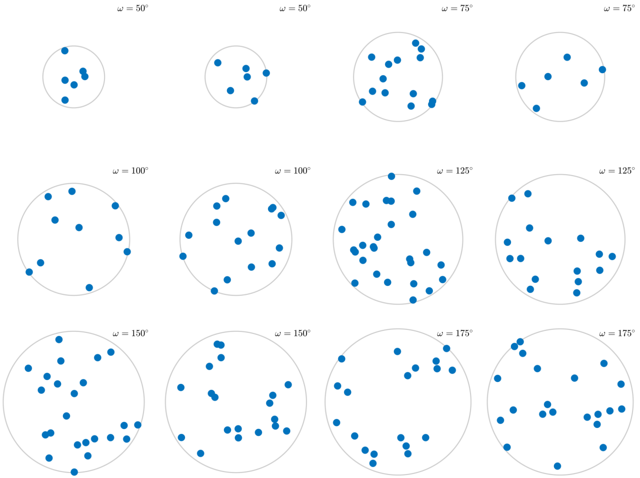

Summary of Rotation Representations

name	notation	space	dimension
matrix	$\mathbf{R}$	$\mathbb{R}^{3\times 3}$	9
Euler angles	$(\varphi_1, \Phi, \varphi_2)$	$[0, 2\pi] \times [0, \pi] \times [0, 2\pi]$	3
quaternion	(q_1, q_2, q_3, q_4)	$\mathbb{S}^4$	4
Rodrigues - Frank	$\tan \frac{\omega}{2} \vec{v}$	$\mathbb{R}^3$	3
axis angle	$\omega \vec{v}$	$\mathbb{B}^3$	3
Miller-Bravais Indices	$(hkl)[uvw]$	$\mathbb{S}^2 \times \mathbb{S}^2$	6

Symmetries

Definition

A symmetry is a transformation that keeps something invariant.

Affine Transformations

Definition

Affine transformations are transformations

$$\mathbf{S}(\vec{x}) = \mathbf{R}\vec{x} + \vec{t}$$

that are compositions of a rotation $\mathbf{R} \in O(3)$ and a translation $\vec{t} \in \mathbb{R}^3$.

The set of all affine transformations in the three dimensional space is called Euclidean motion group and is denoted by $\mathrm{SE}(3)$.

Let $\mathbf{S}_1(\vec{x}) = \mathbf{R}_1\vec{x} + \vec{t}_1$ and $\mathbf{S}_1(\vec{x}) = \mathbf{R}_1\vec{x} + \vec{t}_1$ be two affine transformations. Then their composition

$$\mathbf{S}_2 \circ \mathbf{S}_1(\vec{x}) = \mathbf{S}_2(\mathbf{S}_1(\vec{x})) = \mathbf{R}_2\mathbf{R}_1\vec{x} + \mathbf{R}_2\vec{t}_1 + \vec{t}_2$$

is again an affine transformation.

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is again an affine transformation.

Crystal Symmetries

Definition

The subset $\mathcal{E} \subset \mathrm{SE}(3)$ off all affine transformations that keep the atom lattice invariant is called space group of the crystal.

The space group $\mathcal{S}$ together with the composition $\circ$ is a group, since for any two symmetries $\mathbf{S}_1, \mathbf{S}_2 \in \mathcal{E}$ we have $\mathbf{S}_1 \circ \mathbf{S}_2 \in \mathcal{E}$.

Definition

Let $\mathbf{S}_1, \ldots, \mathbf{S}_n \in SE(3)$ arbitrary affine transformations. Then we denote by $\langle \mathbf{S}_1, \ldots, \mathbf{S}_n \rangle$ the smallest subgroup of $SE(3)$ that contains the transformations $\mathbf{S}_1, \ldots, \mathbf{S}_n$ and call it the group generated by $\mathbf{S}_1, \ldots, \mathbf{S}_n$.

Example

The group generated by the rotation $\mathbf{R}_{\vec{z},120^\circ}$ about 120° about the z-axis is

$$\left\langle \mathbf{R}_{\vec{z},120^\circ} \right\rangle = \{\mathbf{R}_{\vec{z},120^\circ}, \mathbf{R}^2_{\vec{z},120^\circ}, \mathbf{R}^3_{\vec{z},120^\circ}\} = \{\mathbf{R}_{\vec{z},0^\circ}, \mathbf{R}_{\vec{z},120^\circ}, \mathbf{R}_{\vec{z},240^\circ}\}$$

Crystal Symmetries

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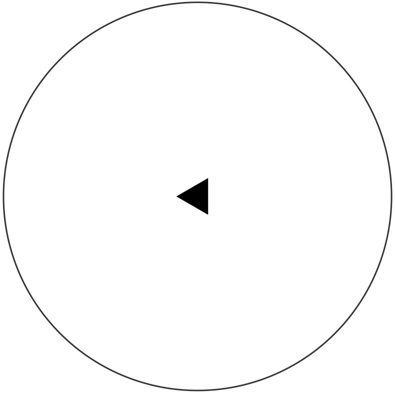
Generate Point Groups in MTEX

```
Z   = vector3d.Z
rot = rotation.byAxisAngle(Z, 120*degree)
cs  = crystalSymmetry.byElements(rot)
```

```
cs.rot = rotation
  size: 3 x 1

  Bunge Euler angles in degree
  phi1  Phi  phi2  Inv.
   240    0     0     0
   120    0     0     0
     0    0     0     0
```



Generate Point Groups in MTEX

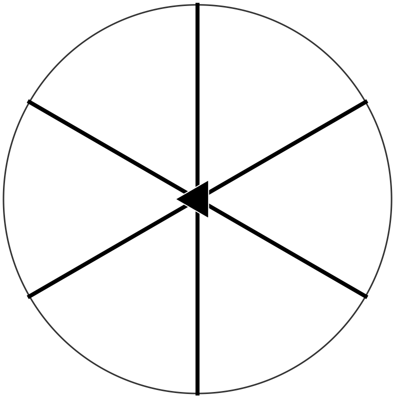
```
Z   = vector3d.Z
rot = rotation.byAxisAngle(Z, 120*degree)
cs  = crystalSymmetry.byElements(rot)
```

add some mirroring

```
m  = reflection(vector3d.X)
cs = crystalSymmetry.byElements([rot, m])
```

```
cs.rot = rotation
  size: 6 x 1

  Bunge Euler angles in degree
  phi1  Phi phi2 Inv.
   240  180    0    1
     0  180  240    1
   120  180  120    1
   240    0    0    0
   120    0    0    0
     0    0    0    0
```



Generate Point Groups in MTEX

```
Z   = vector3d.Z
rot = rotation.byAxisAngle(Z, 120*degree)
cs  = crystalSymmetry.byElements(rot)
```

add some mirroring

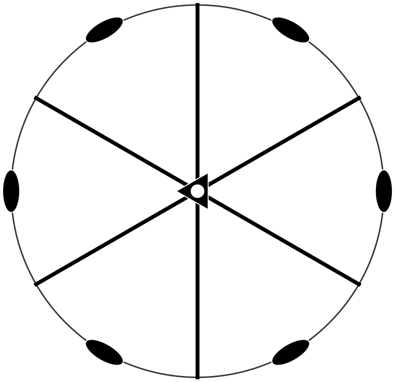
```
m  = reflection(vector3d.X)
cs = crystalSymmetry.byElements([rot, m])
```

add the inversion

```
cs = cs.add(rotation.inversion)
```

```
cs = crystalSymmetry

  symmetry       : -3m1
  elements       : 12
  a, b, c        : 1, 1, 1
  reference frame: X||a, Y||b, Z||c
```



Generate Point Groups in MTEX

```
Z   = vector3d.Z
rot = rotation.byAxisAngle(Z, 120*degree)
cs  = crystalSymmetry.byElements(rot)
```

add some mirroring

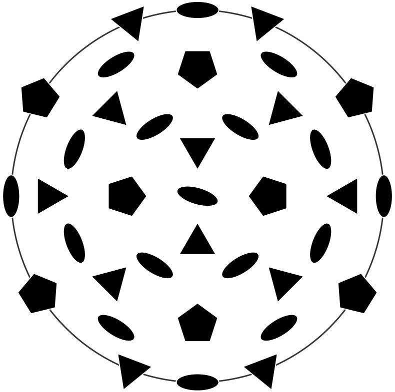
```
m  = reflection(vector3d.X)
cs = crystalSymmetry.byElements([rot, m])
```

add the inversion

```
cs = cs.add(rotation.inversion)
```

some quasi symmetry

```
r2 = rotation.byAxisAngle(Z, 180*degree)
a5 = vector3d.byPolar(31.7171*degree, 0)
r5 = rotation.byAxisAngle(a5, 72*degree)
cs = crystalSymmetry.byElements([r2, r5])
```



Point Groups

Definition

Let $\mathcal{E} = \{(\mathbf{R}_1, \vec{t}_1), (\mathbf{R}_2, \vec{t}_2), \ldots\}$ be the space group of a crystal structure. Then $\mathcal{P} = \{\mathbf{R}_1, \mathbf{R}_2, \ldots\}$ is a subgroup of $O(3)$ and called the point group of the crystal structure.

- The space group describes the symmetries of an infinite periodic crystal lattice.
- The point group describes the symmetries of the finite unit cell.

Goal:

Characterize and describe all possible space groups $\mathcal{E}$ and all possible point groups $\mathcal{P}$.

Result:

There are exactly 230 different space groups and 32 different point groups.

Point Groups

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- The space group describes the symmetries of an infinite periodic crystal lattice.
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Characterize and describe all possible space groups $\mathcal{E}$ and all possible point groups $\mathcal{P}$.

Result:

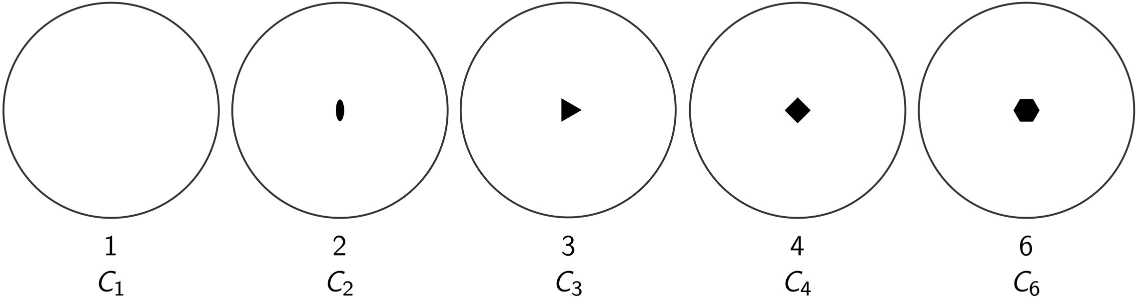
There are exactly 230 different space groups and 32 different point groups.

Symmetry Operations

name	affine transformation	Hermann–Mauguin symbol	graphical symbol
rotational axis	$\mathbf{R}_{\vec{d},\frac{360^\circ}{n}}$	2, 3, 4 ,6	
inversion	$-\mathbf{I}$	$\overline{1}$	
mirror plane	$-\mathbf{R}_{\vec{n},180}$	$m = \overline{2}$	
rotoinversion axis	$-\mathbf{R}_{\vec{d},\frac{360^\circ}{n}}$	$\overline{3}$, $\overline{4}$, $\overline{6}$	
translation	$\vec{t}$		
screw axis	$\mathbf{R}_{\vec{d},\frac{360^\circ}{n}} + \vec{d}$	2_1, 3_1, 3_2, 4_1,4_2,4_3 6_1,6_2,6_3,6_4,6_5	
glide plane	$-\mathbf{R}_{\vec{d},\frac{180^\circ}{n}} + \vec{d}$	a, b, c, n, d	

Cyclic Groups

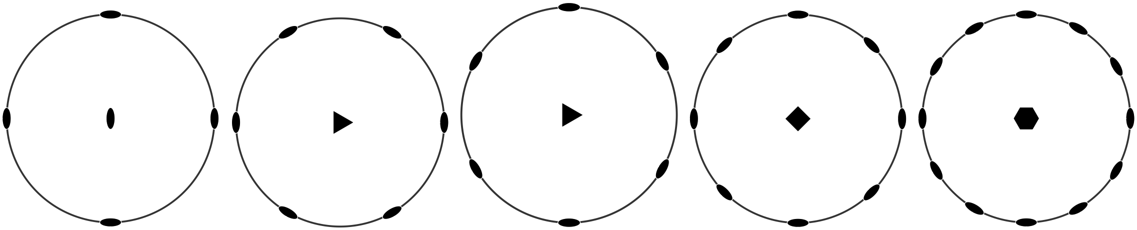
- $\mathbf{S} \in \mathcal{P} \implies \mathbf{S}^n \in \mathcal{P}$, for all $n \in \mathbb{Z}$
- $\mathbf{R}_{\vec{d},\frac{1}{m}360^\circ} \in \mathcal{P} \implies \mathbf{R}_{\vec{d},\frac{n}{m}360^\circ} \in \mathcal{P}$, $n = 0, \ldots, m-1$.
- Only rotational axes of order 2, 3, 4, 6 are compatible with periodic lattices



Dieder Groups

Two two fold symmetry axis $\vec{a}$, $\vec{b}$ at an angle generate a perpendicular symmetry axis

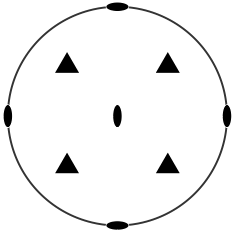
- $\mathbf{R}_{\vec{a},\pi}, \mathbf{R}_{\vec{b},\pi} \in \mathcal{P}$, $\measuredangle(\vec{a},\vec{b}) = \frac{\pi}{n} \implies \mathbf{R}_{\vec{a}\times\vec{b},\frac{2\pi}{n}} \in \mathcal{P}$



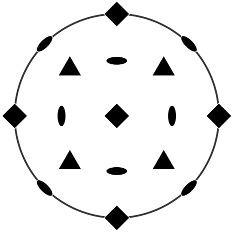
222	321	312	422	622
D_2	D_3	D_3	D_4	D_6

Tetragonal and Cubic Symmetry

- $\vec{a}$ - m-fold symmetry axis, $m > 2$
- $\vec{b}$ - n-fold symmetry axis
- $\implies \mathbf{R}_{\vec{a},\frac{k}{m}2\pi}\vec{b},\ k = 1,\ldots,m$ are n-fold symmetry axes
- $\implies \mathbf{R}_{\vec{b},\frac{k}{n}2\pi}\vec{a},\ k = 1,\ldots,n$ are m-fold symmetry axes
- $\implies \mathbf{R}_{\vec{b},\frac{2k+1}{2n}2\pi}\vec{a},\ k = 0,\ldots,n$ are 2-fold symmetry axes
- assume $\vec{a}$, $\vec{b}$ have minimum angle in $\mathcal{P}$
- $\implies \mathbf{R}_{\vec{a},\frac{k}{m}2\pi}\vec{b},\ k = 1,\ldots,m$ form a regular spherical polygon $P_{\vec{a}}$
- applying all symmetry operations of $\mathcal{P}$ to $P_{\vec{a}}$ will cover the whole sphere by disjoint copies of $P_{\vec{a}}$
- $\implies$ the copies of $P_{\vec{a}}$ form a Platonic solid
- $\implies$ only tetrahedron and cube (octahedron) are relevant

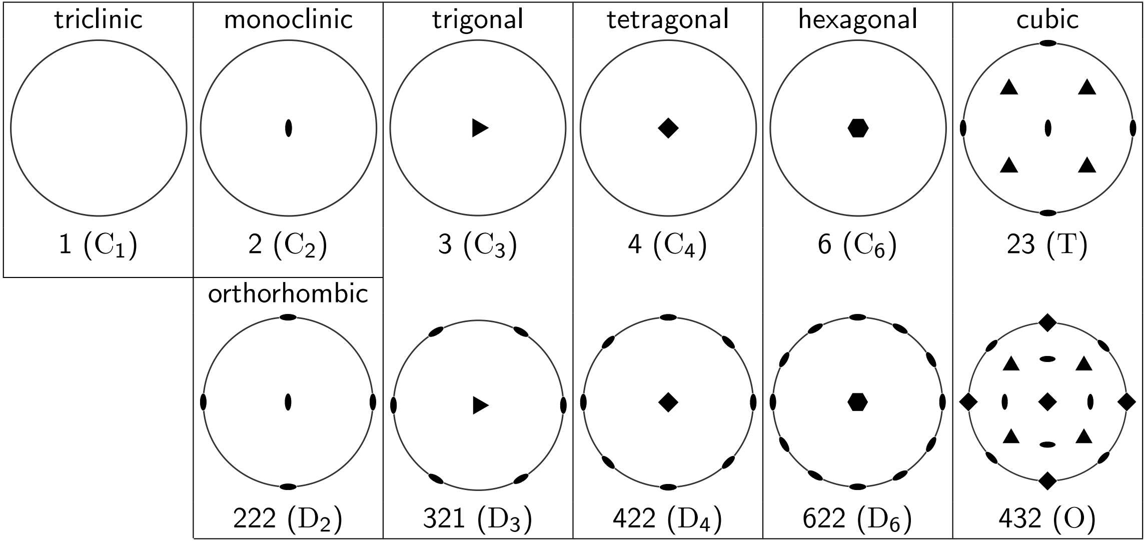


23 (T)

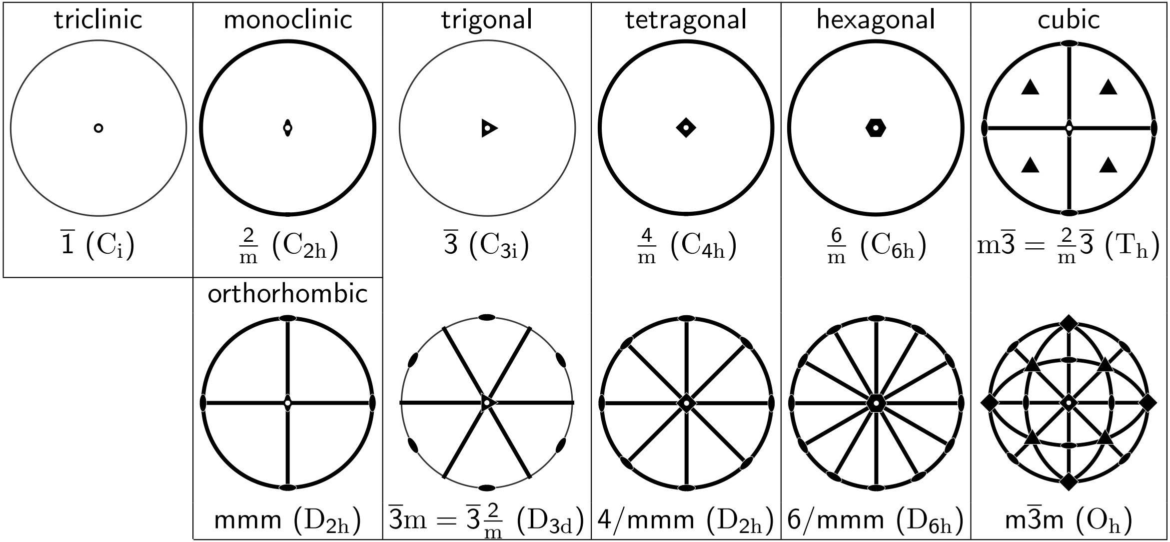


432 (O)

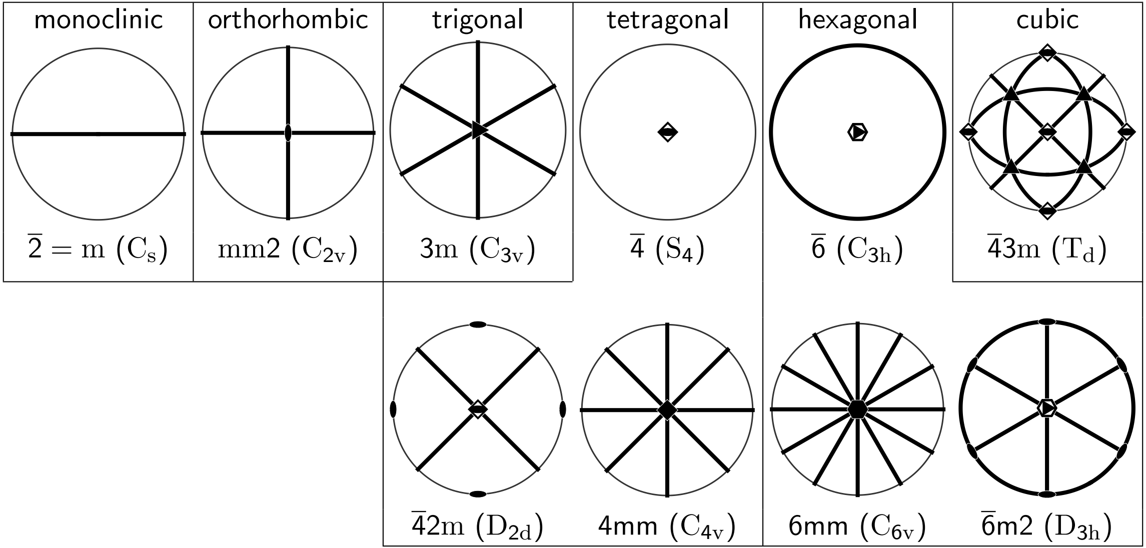
All 11 Enantiomorphic Symmetry Groups



All 11 Laue Symmetry Groups



10 mixed groups



Summary Symmetry Groups

- 11 purely rotational (enatiomorphic) groups:
  - used in most software,
  - only proper rotations are considered
- 11 Laue groups (with inversion center, centrosymmetric groups):
  - correct models for most diffraction experiments, e.g. X-ray diffraction, EBSD
  - only few physical properties are not centrosysmmetric e.g., piezoelectricity
- 10 mixed groups
  - without inversion center
  - each with equally many proper and improper symmetry elements
- 32 different point groups
  - do not represent actual symmetries of the atom lattice - only modulu translation
- 230 different point groups
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Defining Crystal Symmetries in MTEX

```
cs = crystalSymmetry('m-3m')   % by international symbol
cs = crystalSymmetry('Oh')     % by Schoenflies notation
cs = crystalSymmetry('Fm-3m')  % by space group

% import CIF file
cs = crystalSymmetry.load('quartz.cif')

% download from Crystallography Open Database
cs = crystalSymmetry.load('5000036')
```

```
cs.properGroup
cs.Laue
cs.rot
```

```
plotb2east
plot(cs)
```

The 14 Bravais lattices

Question: Which lattices are compatible with the symmetry groups?

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Compatibility with the points groups leads to the 7 crystal systems:

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- monoclinic
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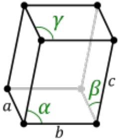
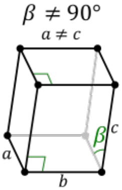
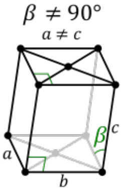
Compatibility with the space groups leads to the the 14 Bravais lattices which additionally separates how the atoms are aligned with the lattice points:

- primitive
- base centered
- body centered
- face centered

<table>
<tr><th>system</th><th>P (primitive)</th><th>C (base centered)</th><th>I (body centered)</th><th>F (face centered)</th></tr>
<tr><td>triclinic
$a \neq b \neq c$,
$\alpha \neq \beta \neq \gamma$</td><td>
</td><td></td><td></td><td></td></tr>
<tr><td>mononclinic
$a \neq b \neq c$,
$\alpha = \gamma = 90^\circ$
$\beta > 90^\circ$</td><td>
</td><td>
</td><td></td><td></td></tr>
<tr><td>orthorhombic
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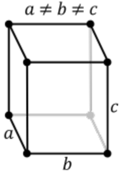
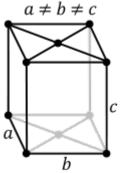
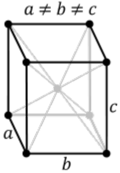
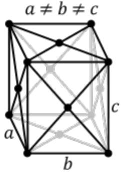
$\alpha = \beta = 90^\circ$
$\gamma = 90^\circ$</td><td>
</td><td>
</td><td>
</td><td>
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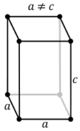
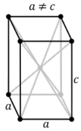
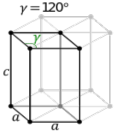
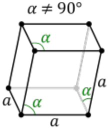
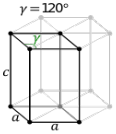
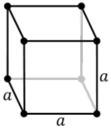
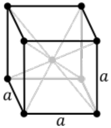
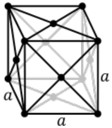
system	P (primitive)	C (base centered)	I (body centered)	F (face centered)
tetragonal $a = b \neq c$, $\alpha = \beta = 90^\circ$ $\gamma = 90^\circ$				
trigonal $a = b \neq c$, $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$				
hexagonal $a = b \neq c$, $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$				
cubic $a = b = c$, $\alpha = \beta = 90^\circ$ $\gamma = 90^\circ$				

A Practical Example

- checkout `https://materialsproject.org/materials/mp-2657/#`
- download cif file

The Ambiguity of the Crystal Coordinate System

the axes of the crystal coordinate system $\vec{a}$, $\vec{b}$, $\vec{c}$ are always chosen such that

- the translations $\mathbf{T}_{\vec{a}}$, $\mathbf{T}_{\vec{b}}$, $\mathbf{T}_{\vec{c}}$ are symmetry elements of the space group
- $\vec{c}$ is the axis of highest symmetry (except for monoclinic and 23)
- $\vec{a}$ or $\vec{b}$ are aligned with the symmetry axes perpendicular to $\vec{c}$

critical symmetries

monoclinic	alignment of the two fold axis: 211, 121, 112, $m11$, $1m1$, $11m$,
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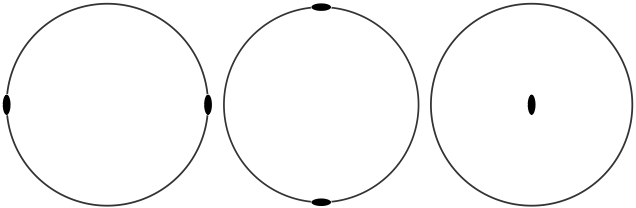

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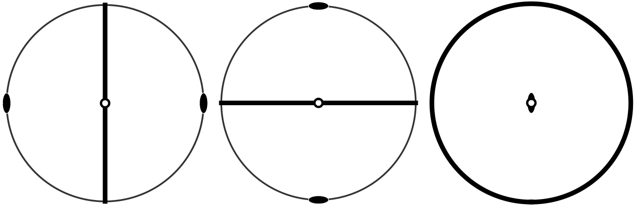

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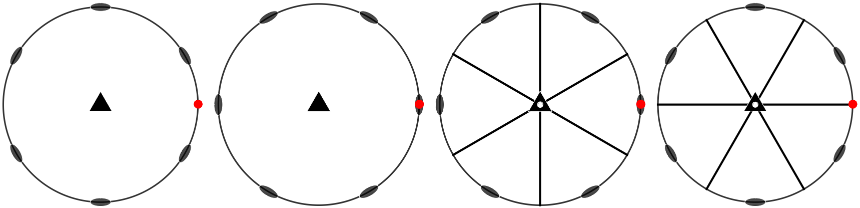

Symmetrically Equivalent Lattice Directions

The crystal axes $\vec{a}$, $\vec{b}$, $\vec{c}$ can be well defined modulo actions of the symmetry group $\mathcal{S}$.

The axes $(\vec{a}, \vec{b}, \vec{c})$ and $(\mathbf{S}\vec{a}, \mathbf{S}\vec{b}, \mathbf{S}\vec{c})$ are physically indistinguishable for all $\mathbf{S} \in \mathcal{S}$

Two lattice directions

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are called symmetrically equivalent if there is a symmetry operations $\mathbf{S} \in \mathcal{S}$ such that

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- $\langle uvw \rangle$ denotes the set of all lattice directions symmetrically equivalent to $[uvw]$
- $\langle uvw \rangle$ may contain at maximum $|\mathcal{S}|$ different lattice directions
- rotational axes have fewer symmetrically equivalent crystal directions, e.g. $\langle 001 \rangle = [001]$
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Symmetrically Equivalent Lattice Planes

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monoclinic: $\langle uvw \rangle = \langle \overline{u} v \overline{w} \rangle$

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cubic: $\langle uvw \rangle = \langle vwu \rangle = \langle wuv \rangle = \langle u \overline{v}\overline{w} \rangle = \langle v \overline{w}\overline{u} \rangle = \langle w \overline{u}\overline{v} \rangle =$
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reference system	single	symmetrically equivalent
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tetragonal: $\langle uvw \rangle = \langle \overline{v} uw \rangle = \langle \overline{u}\, \overline{v} w \rangle = \langle v \overline{u} w \rangle$

cubic: $\langle uvw \rangle = \langle vwu \rangle = \langle wuv \rangle = \langle u \overline{vw} \rangle = \langle v \overline{wu} \rangle = \langle w \overline{uv} \rangle =$
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Analogously the class of symmetrically equivalent lattice planes $\{hk\ell\}$ is defined as the set of all lattice planes $(h_2 k_2 \ell_2)$ such that there is a symmetry operation $\mathbf{S} \in \mathcal{S}$ with

$$(h_2 k_2 \ell_2) = h_2 \vec{a}^* + k_2 \vec{b}^* + \ell_2 \vec{c}^* = \mathbf{S}(h\vec{a}^* + k\vec{b}^* + \ell\vec{c}^*)$$

reference system	single	symmetrically equivalent
lattice point	$\cdot uvw \cdot$	$: uvw :$
lattice direction	$[uvw]$	$\langle uvw \rangle$
lattice plane	$(hk\ell)$	$\{hkl\}$

Symmetrically Equivalent Lattice Planes

For most symmetries the symmetrically equivalent directions comes as permutations of the Miller indices

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Miller Indices for Trigonal and Hexagonal Symmetries

For trigonal and hexagonal symmetries symmetrically equivalent directions can **not** be determined by permuting the three digit Miller indies.

Miller Indices for Trigonal and Hexagonal Symmetries

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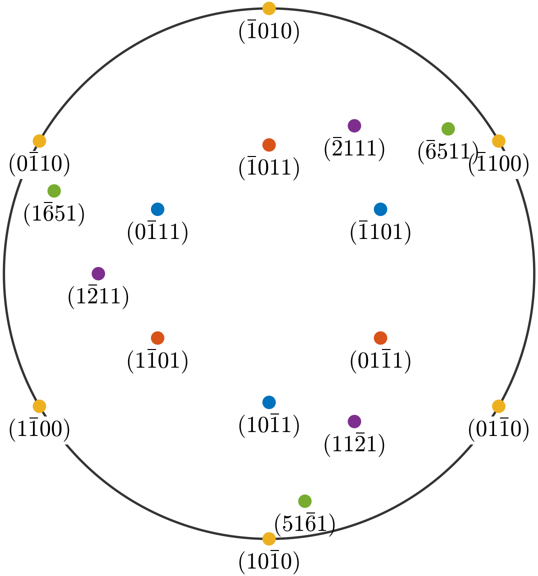
Solution: 4 digit Miller indices

$(HKIL)$ $H = h,\ K = k,\ i = -h - k,\ L = \ell$

$[UVTW]$ $U = 2u - v,\ V = 2v - u,$
$T = -u - v,\ W = 3w$



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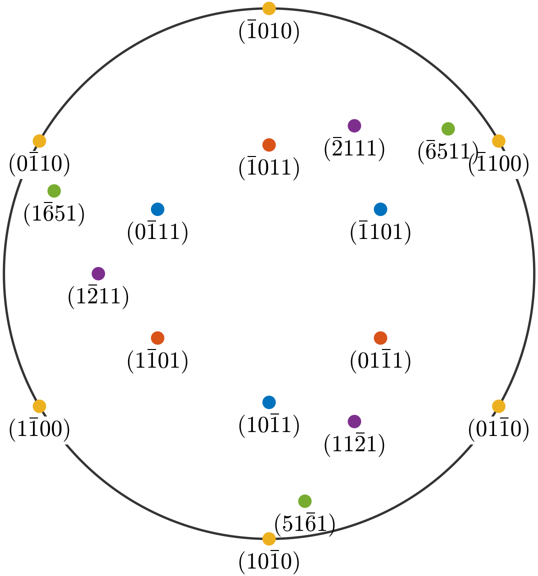

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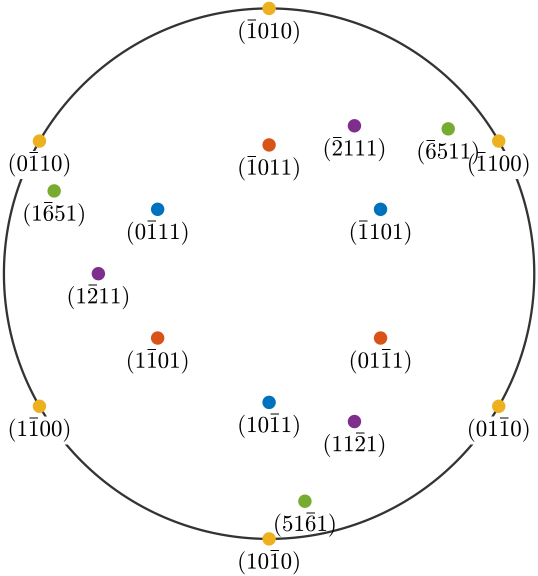


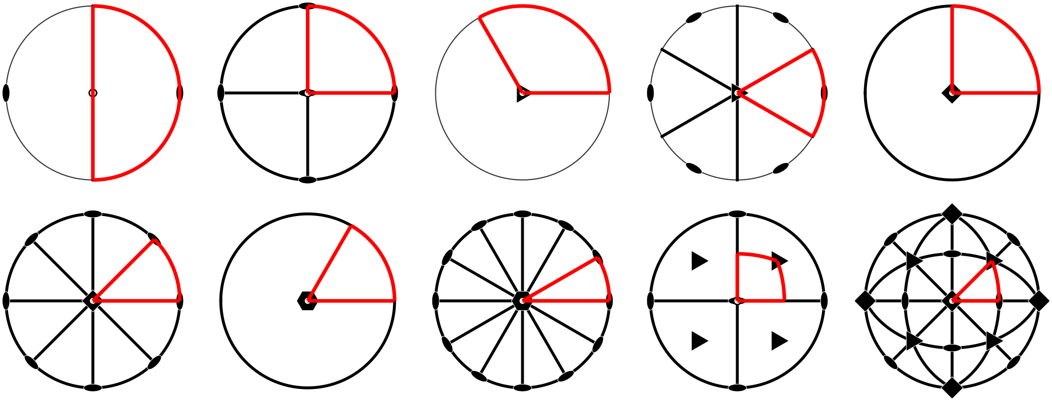
MTEX

```
% define some crystal direction
cs = crystalSymmetry('321',[4.9 4.9 5.4],'mineral','quartz')
h = Miller({1,0,-1,0},{0,0,0,1},cs,'UVTW')

% define some crystal plane
h = Miller({1,0,-1,0},{0,0,0,1},cs,'HKIL')

% find all symmetrically equivalent
hSym = h.symmetrise
unique(h.symmetrise,'noSymmetry')

h.multiplicity

angle(hSym(1),hSym(2))

angle(hSym(1),hSym(2),'noSymmetry')
```

The Fundamental Sector

Definition

The fundamental sector is a spherical region which contains from each class of symmetrically equivalent vectors exactly one.



MTEX

```
% the fundamental sector for a given symmetry
sR = cs.fundamentalSector
plot(sR)

% check whether we are inside the fundamental region
sR.checkInside(h)

% define some crystal plane
h = Miller({1,0,-1,0},{0,0,0,1},cs,'HKIL')
h = h.project2FundamentalRegion

% generate vectors within a spherical region
r = vector3d.rand(sR)
r = equispacedS2Grid(sR)
```