- There is one-to-one correspondence between object's orientations and rotations.

- An orientation of an object can be represented an orthogonal matrix.

  (Proper) rotations are represented (special) orthogonal matrices.

  Composition of rotations corresponds to multiplication of representing them orthogonal matrices.

- There is two-to-one correspondence between unit quaternions and special orthogonal matrices.

- Rotation/orientation parameterizations:
  - Axis and angle
  - Euler angles
  - Rodrigues parameters

Description of orientations and misorientations in the presence of symmetry

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Outline

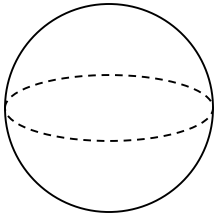
- Crystallographic point groups
- Asymmetric domains
- Misorientation angle distributions
- Misorientation axis distributions

- Symmetry operation – object's configurations w/r to its environment before and after the operation are identical.
- An object is symmetric if there exists a non-trivial symmetry operation.
- Orientation analysis is influenced by objects' symmetries.
- Crystals exhibit symmetries.

- Symmetry operations of an object constitute a group.
- Point group – there exists a point fixed under all symmetry operations of the group.
- Symmetry operations of a point group are rotations.

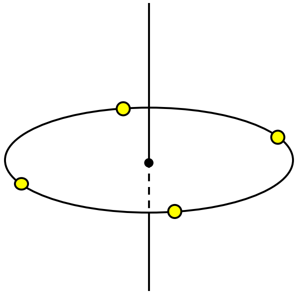
Point groups

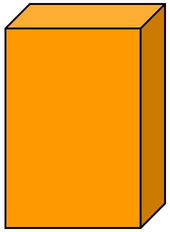
Proper rotations

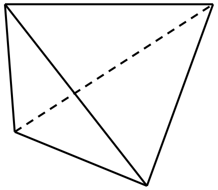


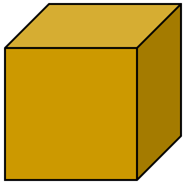
$SO(3)$

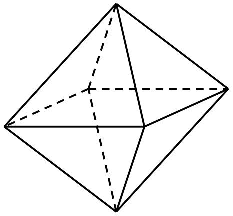
C_n	- the family of cyclic groups
D_n	- the family of dihedral groups
T	- tetrahedral group
O	- octahedral group
I	- icosahedral group





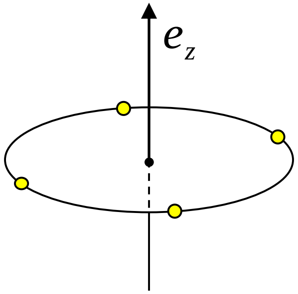






Point groups - example

$$C_4$$

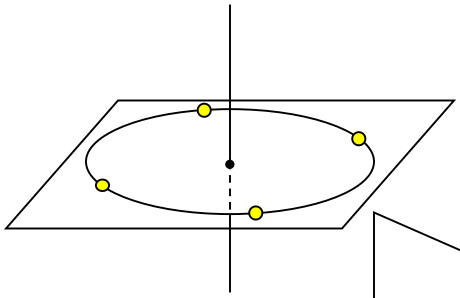


I	$O(e_z, \pi/2)$	$O(e_z, \pi)$	$O(e_z, 3\pi/2)$
$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

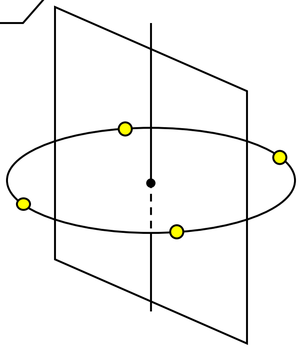
Point groups

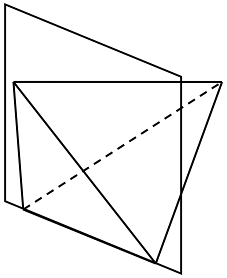
All rotations

$O(3)$



C_{nh}	C_n	+ reflection w/r to h
C_{nv}	C_n	+ reflection w/r to v
S_{2n}	C_n	+ (π/n) & (reflection w/r to h)
D_{nh}	D_n	+ reflection w/r to h
D_{nd}	D_n	+ reflection w/r to d
T_d	T	+ reflection w/r to d
T_h	T	+ inversion
O_h	O	+ inversion
I_h	I	+ inversion





$C_s = C_{1h}$

$C_i = S_2$

Crystallographic point groups

Crystallographic point group = a point group of a lattice

Crystallographic point groups have finite orders.

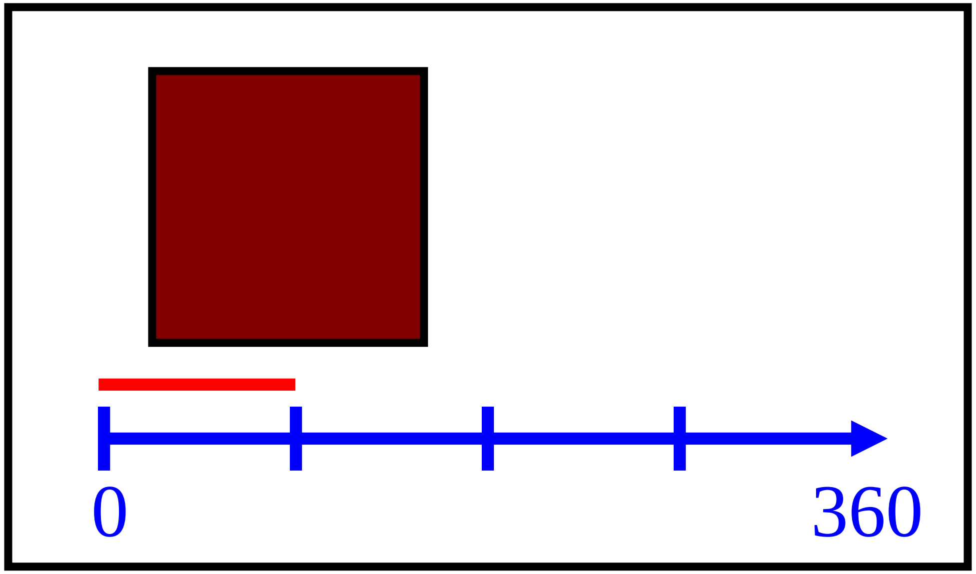
In 3D there are 32 (geometric classes) of crystallographic point groups.

C_1	C_2	C_3	C_4	C_6	D_2	D_3	D_4	D_6	T	O
C_i	C_{2h}	S_6	C_{4h}	C_{6h}	D_{2h}	D_{3d}	D_{4h}	D_{6h}	T_h	O_h
C_s	S_4	C_{3h}	C_{2v}	C_{3v}	C_{4v}	C_{6v}	D_{2d}	D_{3h}	T_d	.

Crystal systems

Triclinic	Monoclinic	Orthorhombic	Trigonal	Tetragonal	Hexagonal	Cubic
C_i	C_{2h}	D_{2h}	D_{3d}	D_{4h}	D_{6h}	O_h
C_1	C_2	D_2	D_3	D_4	D_6	O
		C_{2v}	C_{3v}	C_{4v}	C_{6v}	
	C_s			D_{2d}	D_{3h}	T_d
			S_6	C_{4h}	C_{6h}	T_h
			C_3	C_4	C_6	T
				S_4	C_{3h}	

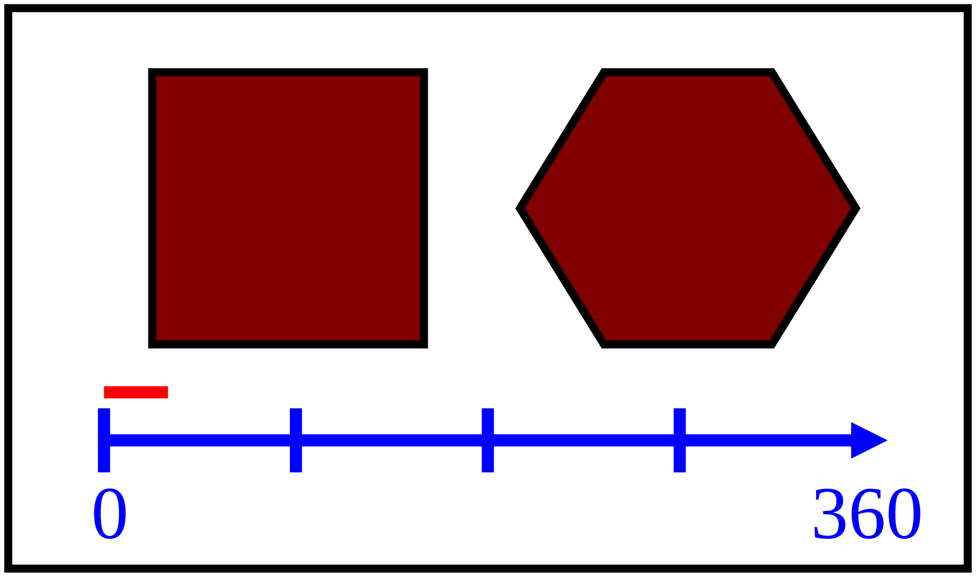
Asymmetric domains



$$\varphi \rightarrow \varphi + k \cdot 90^\circ$$

Asymmetric domain – the smallest closed subset of the orientation space such that symmetrical images of the domain cover the space

Asymmetric domains



$3k+2l$	k	l
0	0	0
1	1	-1
2	0	1
3	1	0
4	0	2
5	1	1
6	2	0
7	1	2
8	2	1
9	3	0
10	2	2
11	3	1

$$\varphi \to \varphi + k \cdot 90^\circ + l \cdot 60^\circ = \varphi + 30^\circ \cdot (3k + 2l)$$

Asymmetric domain – the smallest closed subset of the orientation space such that symmetrical images of the domain cover the space

Asymmetric domains

$$O \quad + \quad \text{Crystal symmetry} \quad - \quad CO$$

Two crystallites: $C_1 O_1, \quad C_2 O_2$

Misorientation

$$C_2 O_2 \left(C_1 O_1 \right)^T = C_2 (O_2 O_1{}^T) C_1{}^T = C_2 O C_1{}^T$$

crystal symmetry ? O ? crystal symmetry $\quad C_2 \times O \times C_1$

---

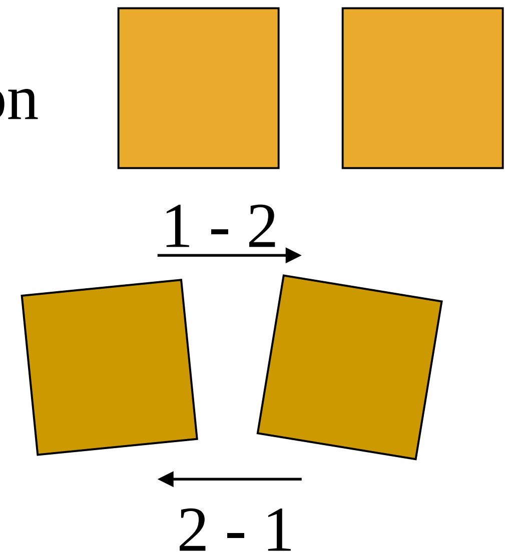
crystal symmetry ? O ? sample symmetry $\quad C \times O \times S$

Asymmetric domains

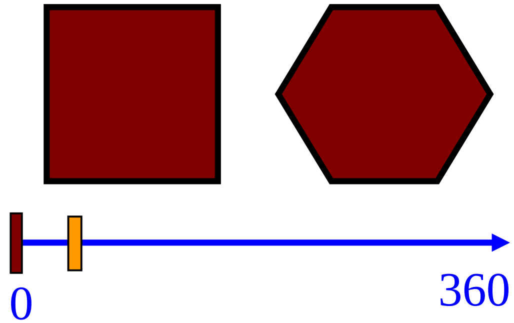
One phase:

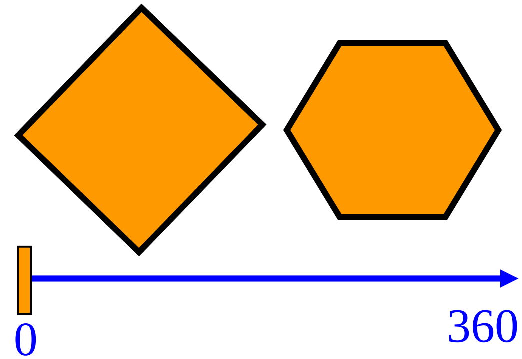
- natural reference misorientation

- additional equivalence
  for indistinguishible objects

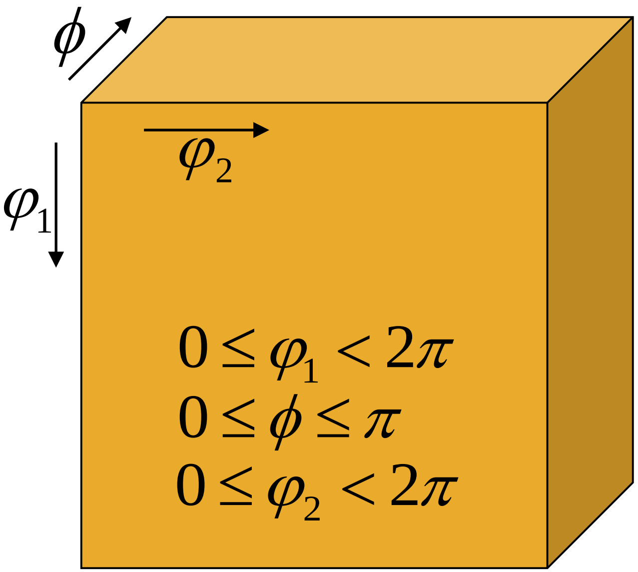


Multi-phase:





Asymmetric domains Euler angles

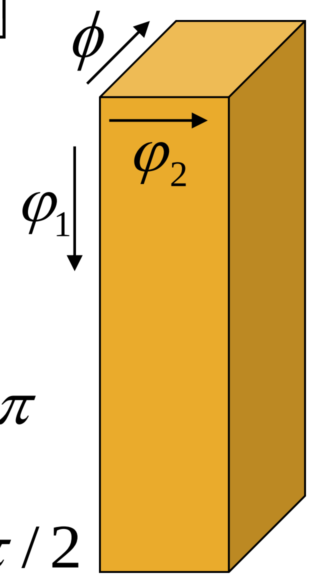


C_4 (tetragonal)

$$(e_z, \pi/2) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$(e_z, \pi/2) \circ O(\varphi_1, \phi, \varphi_2) = O(\varphi_1, \phi, \varphi_2 + \pi/2)$$

$$(\varphi_1, \phi, \varphi_2) \Leftrightarrow (\varphi_1, \phi, \varphi_2 + k\pi/2)$$



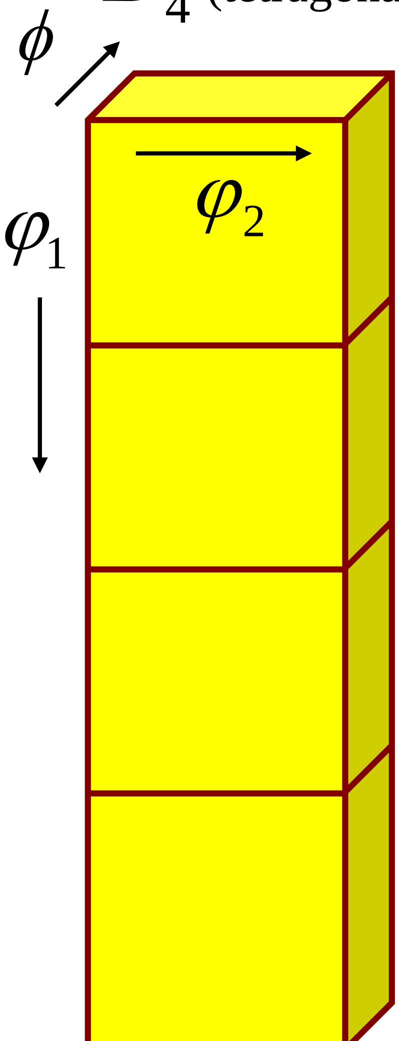
$0 \le \varphi_1 < 2\pi$

$0 \le \phi \le \pi$

$0 \le \varphi_2 < \pi/2$

Asymmetric domains Euler angles

D_4 (tetragonal)

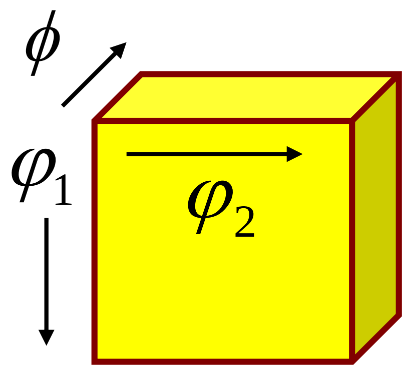


crystal symmetry ? O ? sample symmetry

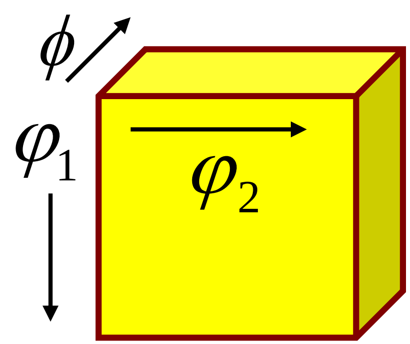
$$C \times O \times S$$

$$D_4 \times D_2$$

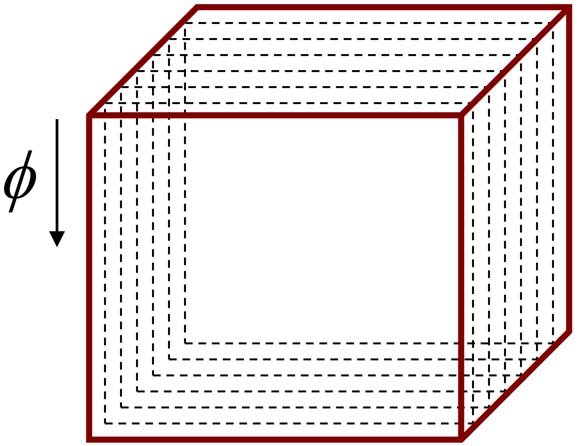
tetragonal - orthorhombic



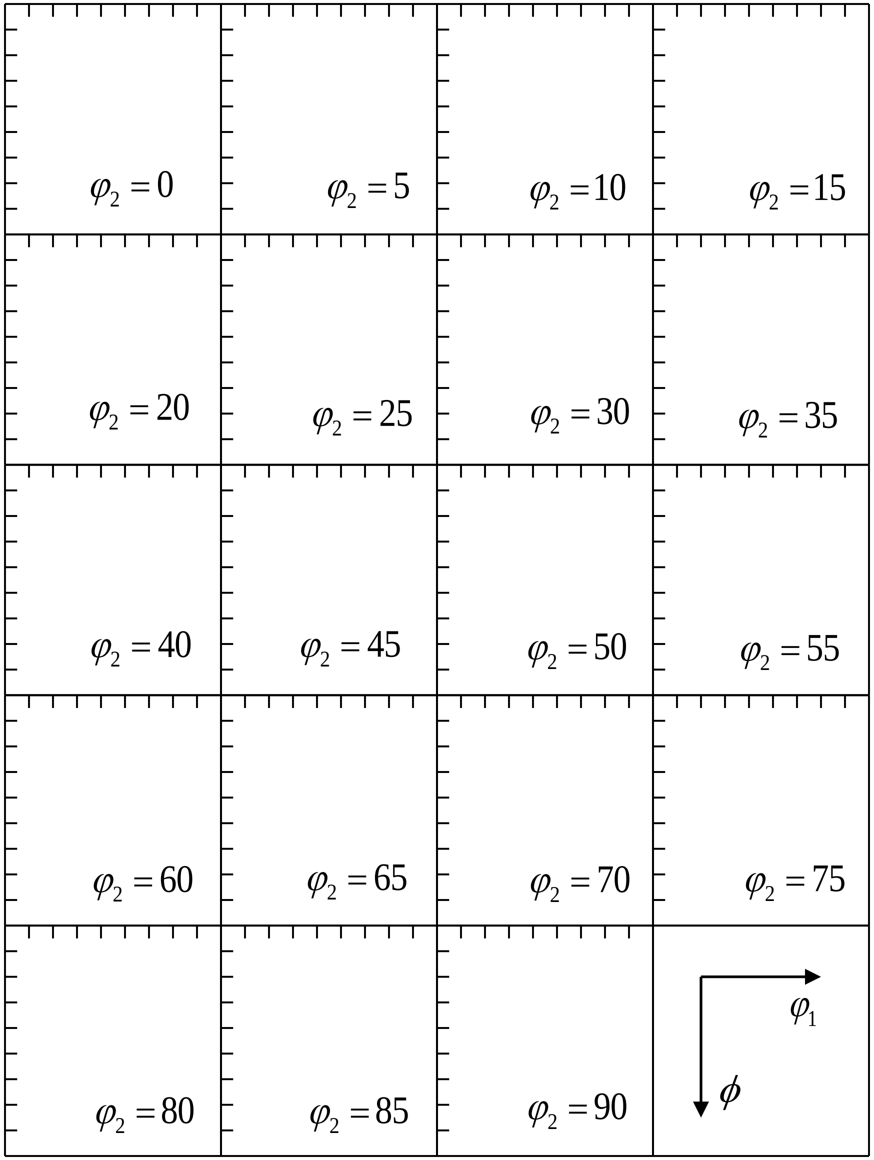
cubic - orthorhombic $O \times D_2$



? **1/3**



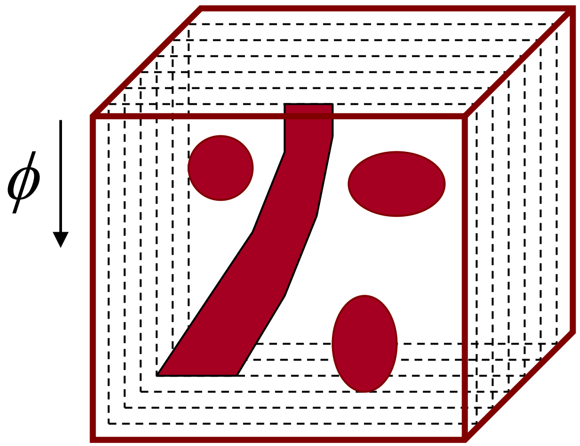
ϕ



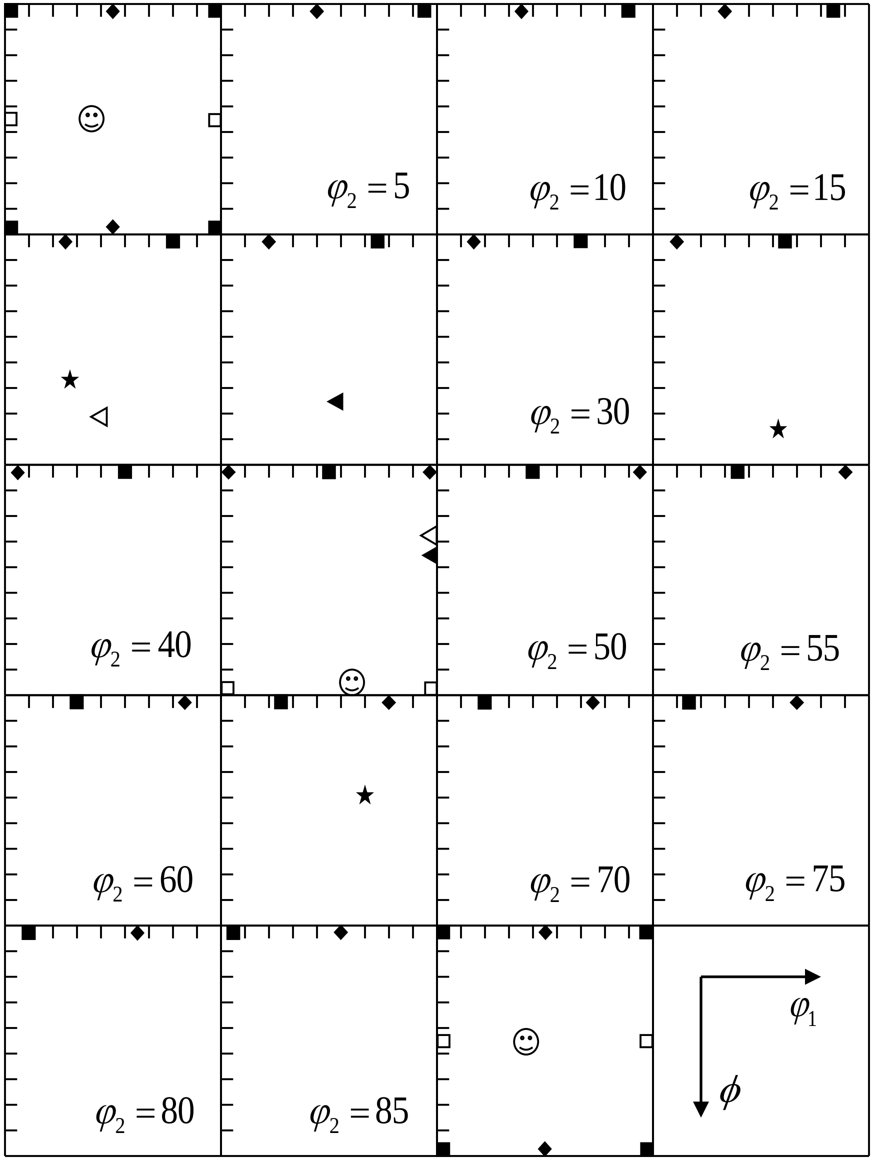
$\varphi_2 = 0$
$\varphi_2 = 5$
$\varphi_2 = 10$
$\varphi_2 = 15$
$\varphi_2 = 20$
$\varphi_2 = 25$
$\varphi_2 = 30$
$\varphi_2 = 35$
$\varphi_2 = 40$
$\varphi_2 = 45$
$\varphi_2 = 50$
$\varphi_2 = 55$
$\varphi_2 = 60$
$\varphi_2 = 65$
$\varphi_2 = 70$
$\varphi_2 = 75$
$\varphi_2 = 80$
$\varphi_2 = 85$
$\varphi_2 = 90$
φ_1
ϕ

Orientation components

$$f = f(\varphi_1, \phi, \varphi_2)$$

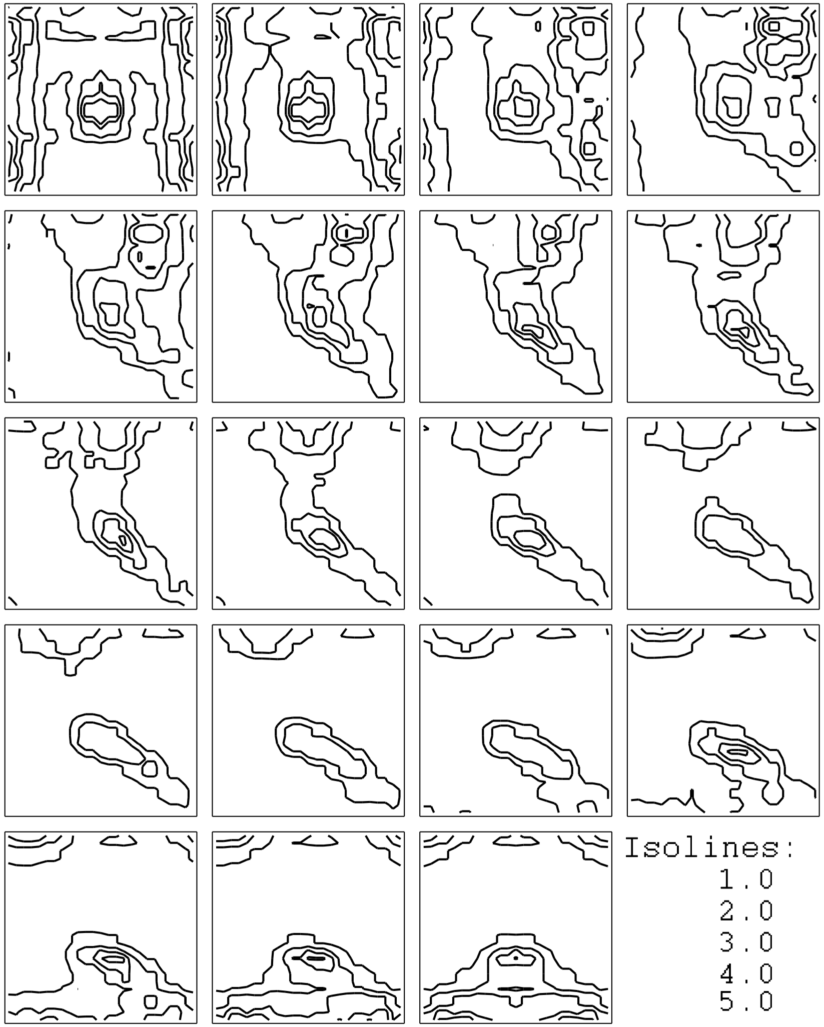


☺ - brass
■ - cube
□ - Goss
◀ - copper
◁ - Dillamore
◆ - shear
★ - S



Example experimental ODF

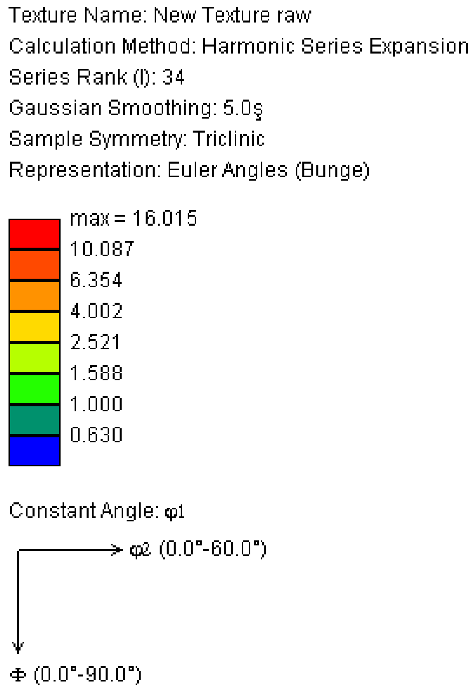
Orientation density function of FeSi after primary recrystalization

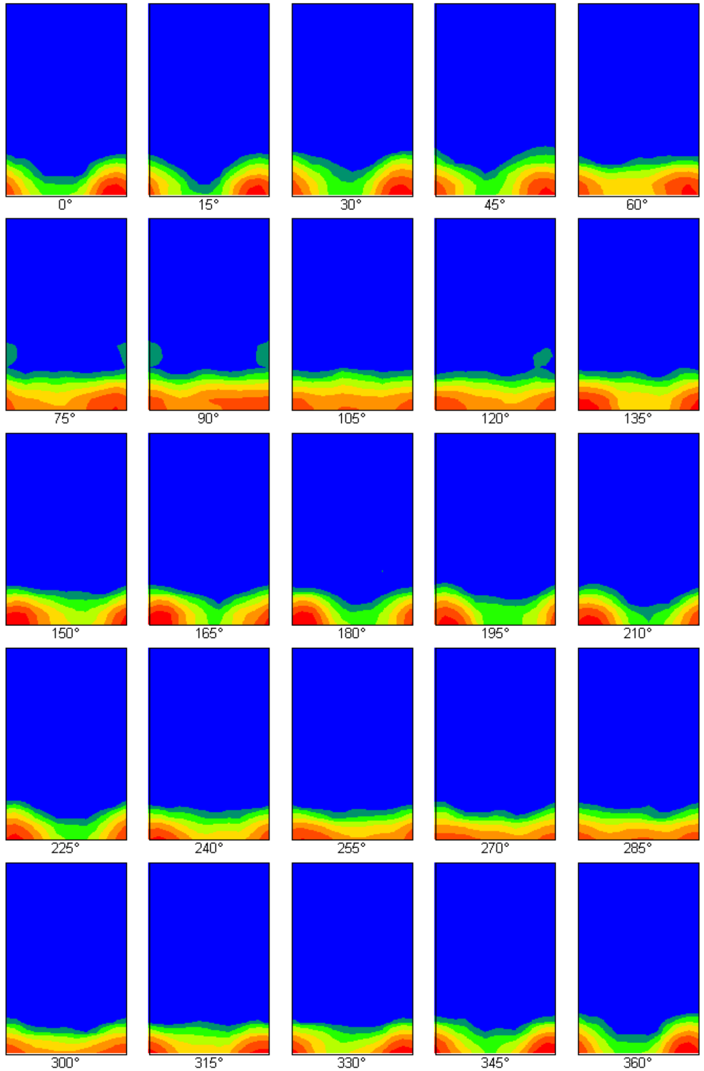


φ_1 projection

Example experimental ODF

Orientation density function of extruded Ti-α (Grade 2)





φ_1 projection

Asymmetric domains Miller indices

Cubic crystal symmetry

Simultaneous permatations in (...) and [...].

Even permatation add even number of '-'.

Odd permatation add odd number of '-'.

(1 2 3)[6 3 -4]	(-3 2 1)[4 3 6]
(2 -1 3)[3 -6 -4]	(-3 -1 2)[4 -6 3]
(2 3 1)[3 -4 6]	(2 -3 -1)[3 4 -6]
(-1 -2 3)[-6 -3 -4]	(1 3 -2)[6 -4 -3]
(3 -2 1)[-4 -3 6]	(-3 1 -2)[4 6 -3]
(-1 3 2)[-6 -4 3]	(3 -1 -2)[-4 -6 -3]
(3 1 2)[-4 6 3]	(-3 -2 -1)[4 -3 -6]
(-2 1 3)[-3 6 -4]	(-1 -3 -2)[-6 4 -3]
(-2 -3 1)[-3 4 6]	(2 1 -3)[3 6 4]
(1 -3 2)[6 4 3]	(-1 2 -3)[-6 3 4]
(-2 3 -1)[-3 -4 -6]	(1 -2 -3)[6 -3 4]
(3 2 -1)[-4 3 -6]	(-2 -1 -3)[-3 -6 4]

Asymmetric domains   Miller indices

Cubic - orthorhombic symmetry

Besides equivalences of cubic crystal symmetry:

(1 2 3)[6 3 -4]

(1 2 -3)[6 3 4]

(1 2 3)[-6 -3 4]

(1 2 -3)[-6 -3 -4]

$\times$ 24

all simultaneous permatations in (...) and [...] +
all sign changes not violating $hu+kv+lw=0$

It is common to omit bars, e.g.,   (1 2 3)[6 3 4]

This does not make sense
when orientations of individual crystallites are considered.

Orientation components

Cubic-orthorhombic symmetry

☺ - brass

■ - cube

□ - Goss

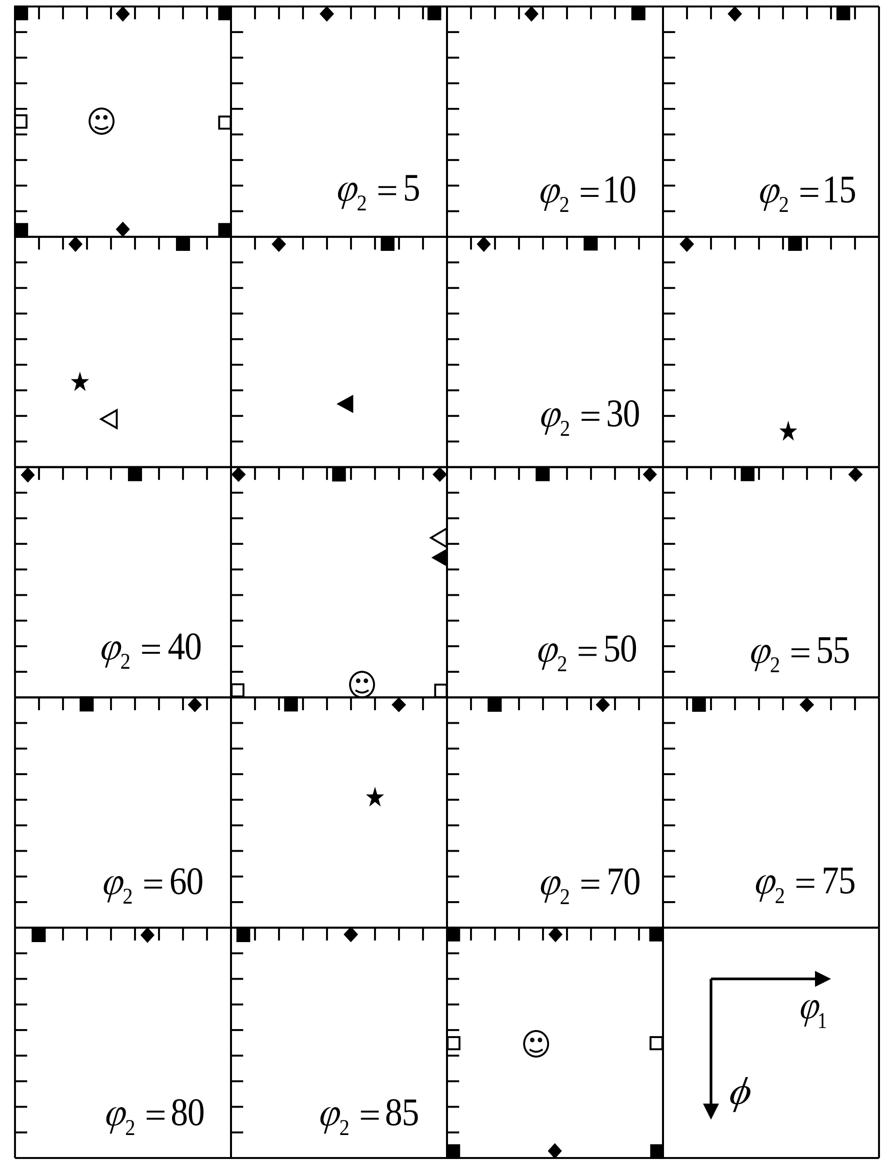
◀ - copper

◁ - Dillamore

◆ - shear

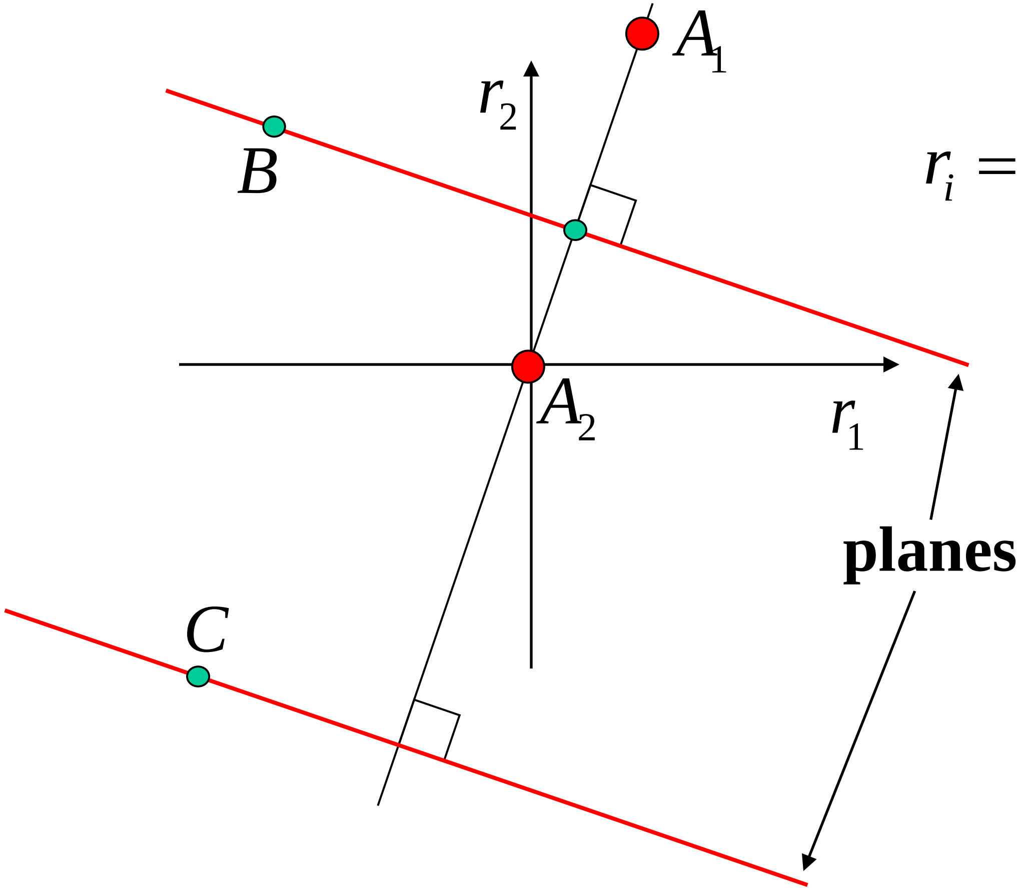
★ - S

	Miller indices
’cube’	(0 0 1) <1 0 0>
’brass’	(0 1 1) <2 1 1>
’copper’	(1 1 2) <1 1 1>
’Goss’	(0 1 1) <1 0 0>
’S’	(2 1 3) <3 6 4>
’shear’	(0 0 1) <1 1 0>
’Dillamore’	(4 4 11) <11 11 8>



Asymmetric domains   Rodrigues space

Rodrigues parameters and orientations
at the same distance to two distinguished orientations



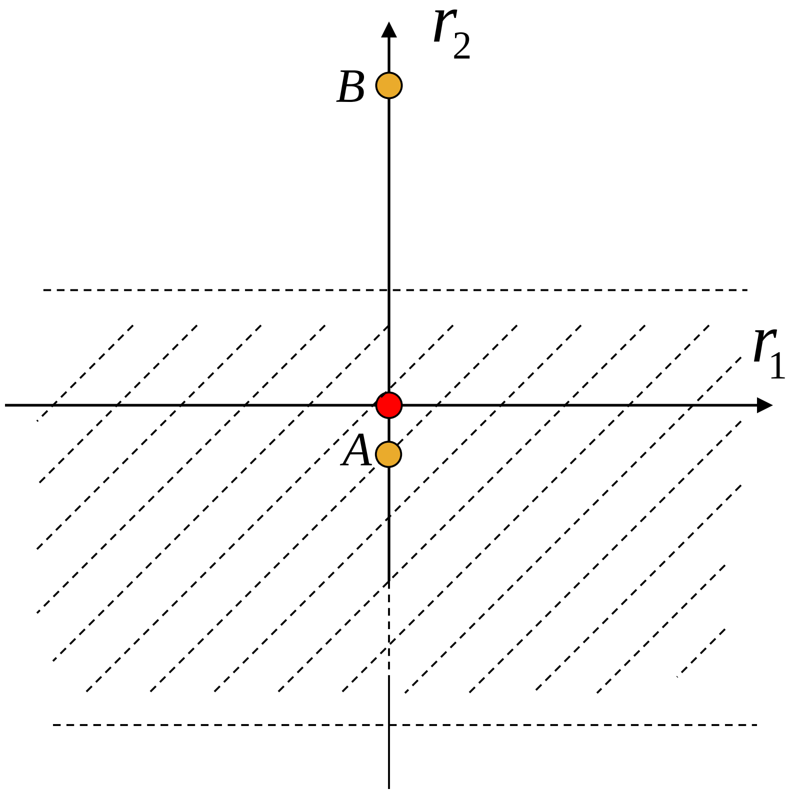
$$r_i = n_i \tan(\omega / 2)$$

$$\omega(A_1, B) = \omega(A_2, B)$$

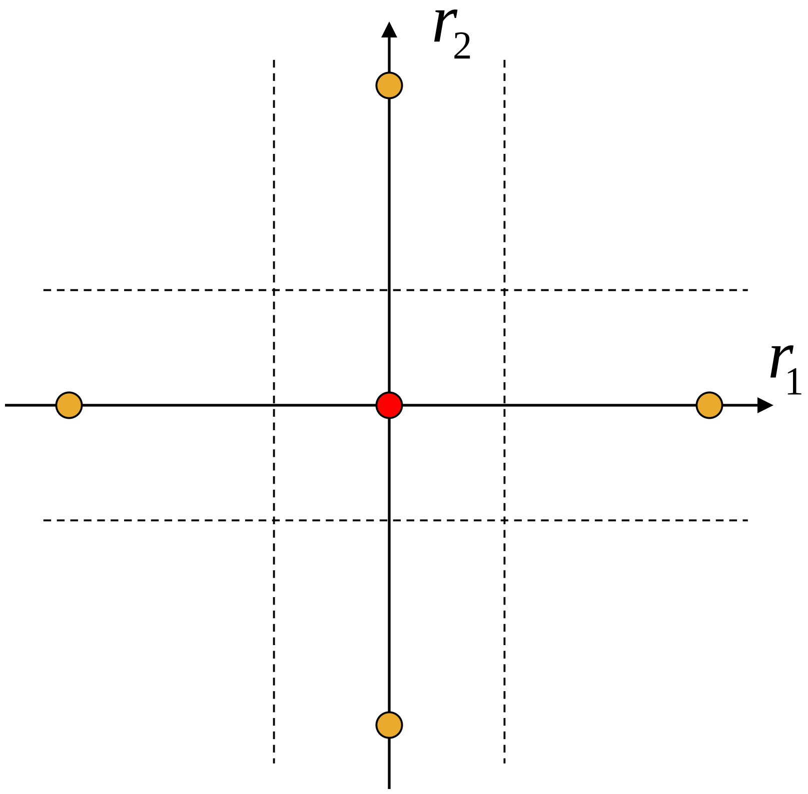
$$\omega(A_1, C) = \omega(A_2, C)$$

Asymmetric domains Rodrigues space

Orientations closer to *A* than to *B*

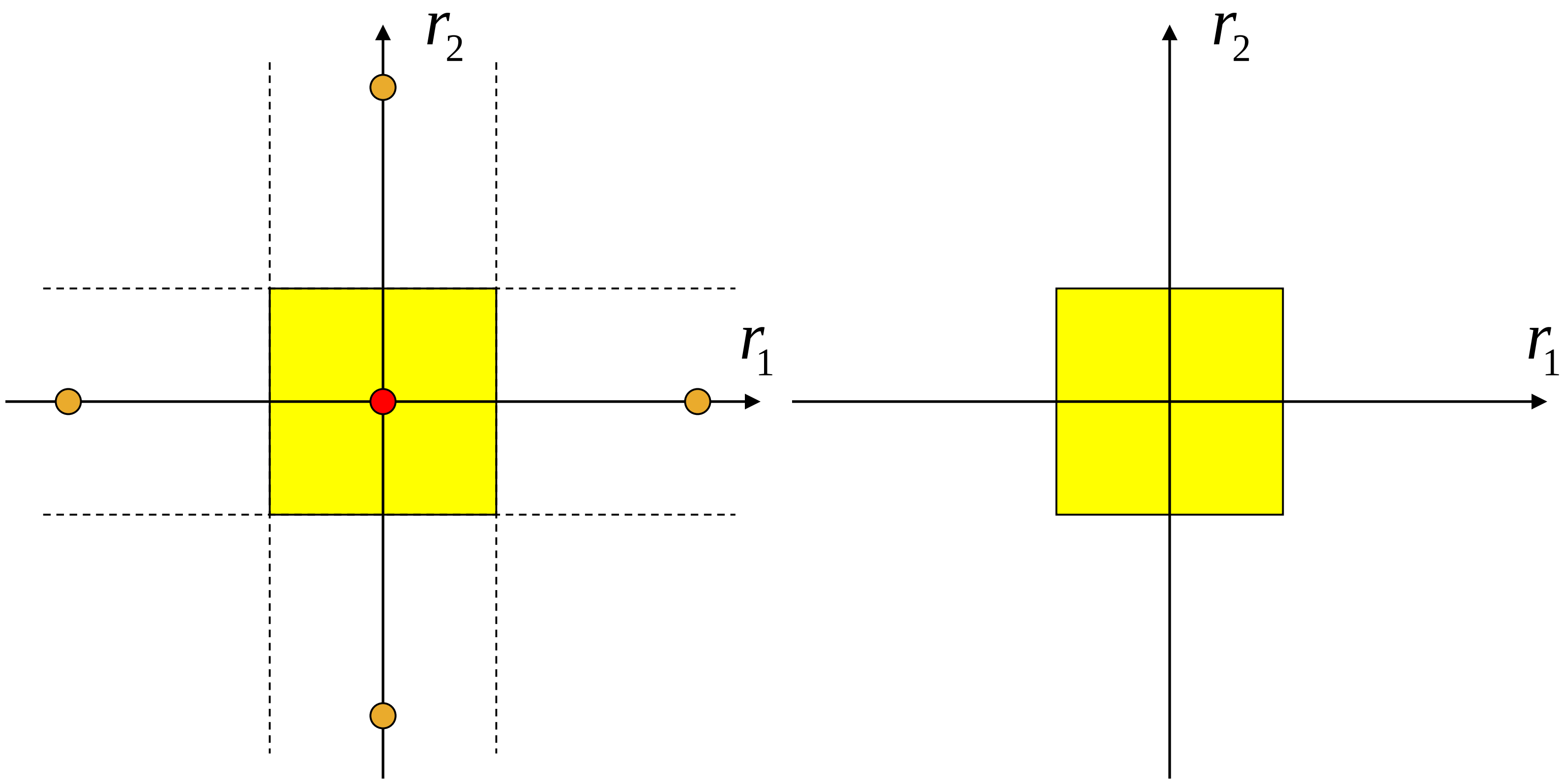


Distinguished points



Asymmetric domains Rodrigues space

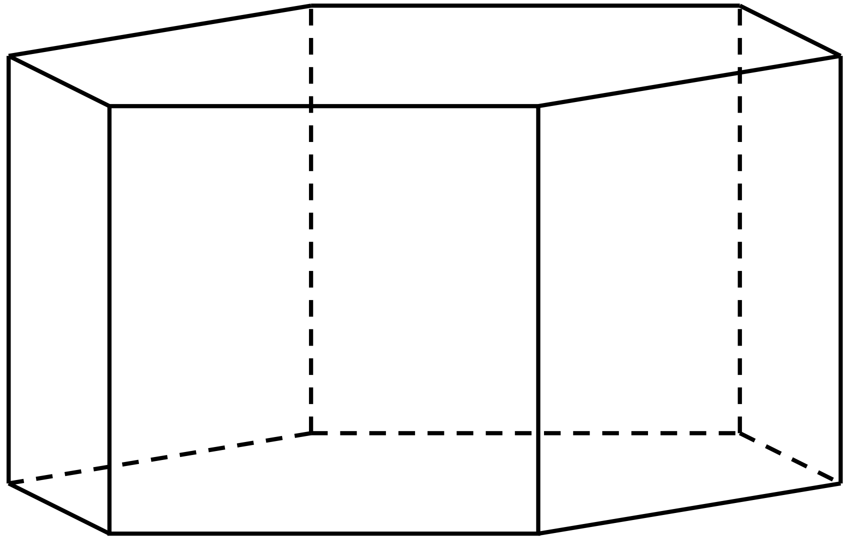
Construction of the asymmetric domain for *CO*



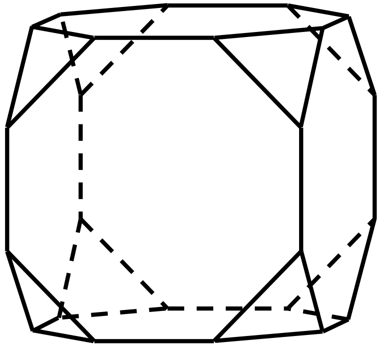
Voronoï cell around *I*

Asymmetric domains   Rodrigues space

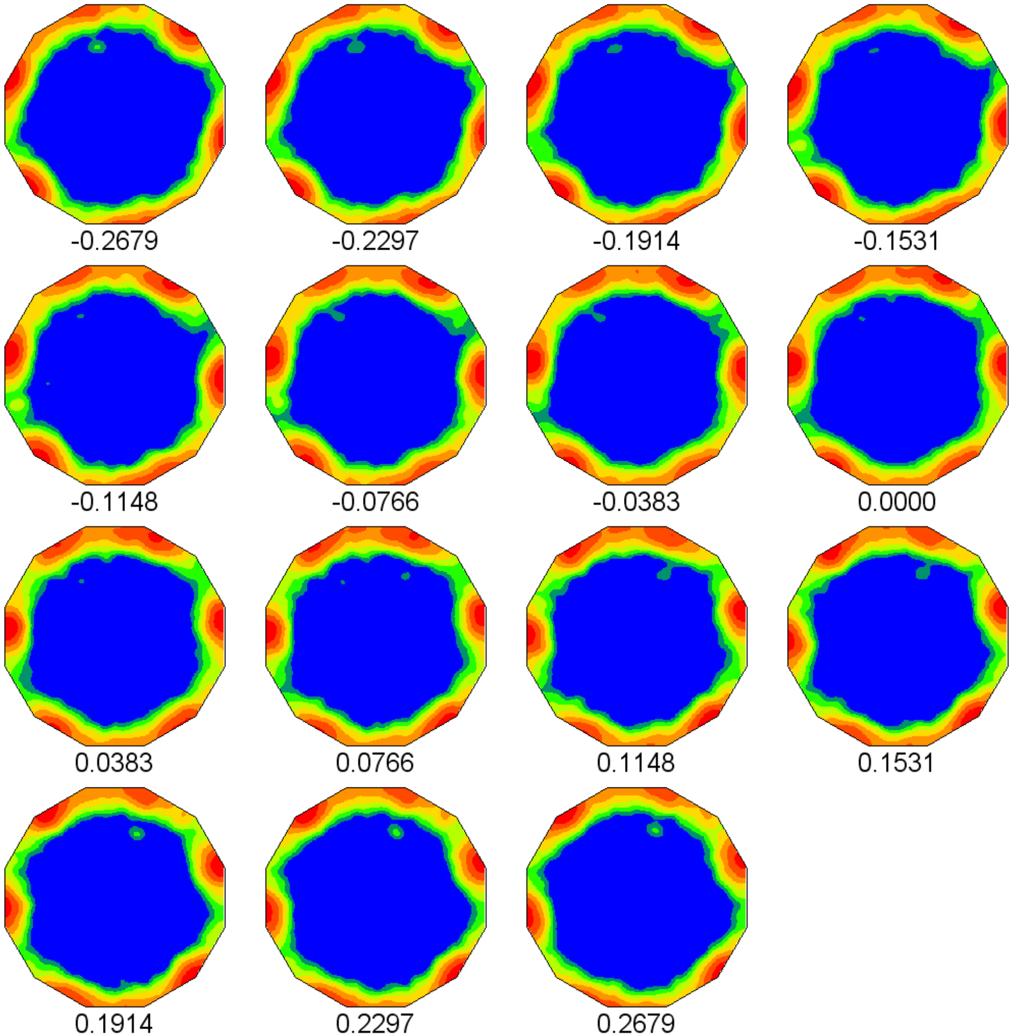
D_3



O



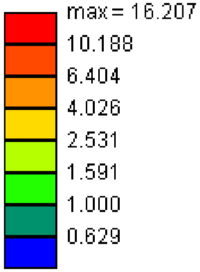
Asymmetric domains, example texture



Extruded Ti-α

D_6

Texture Name: New Texture raw
Calculation Method: Harmonic Series Expansion
Series Rank (l): 34
Gaussian Smoothing: 5.0ş
Sample Symmetry: Triclinic
Representation: Rodrigues Vector



Asymmetric domains Rodrigues space

Domains in the case $C_2 O C_1$

1. No <u>common symmetry operations</u>

   Voronoï cell around I = asymmetric domain

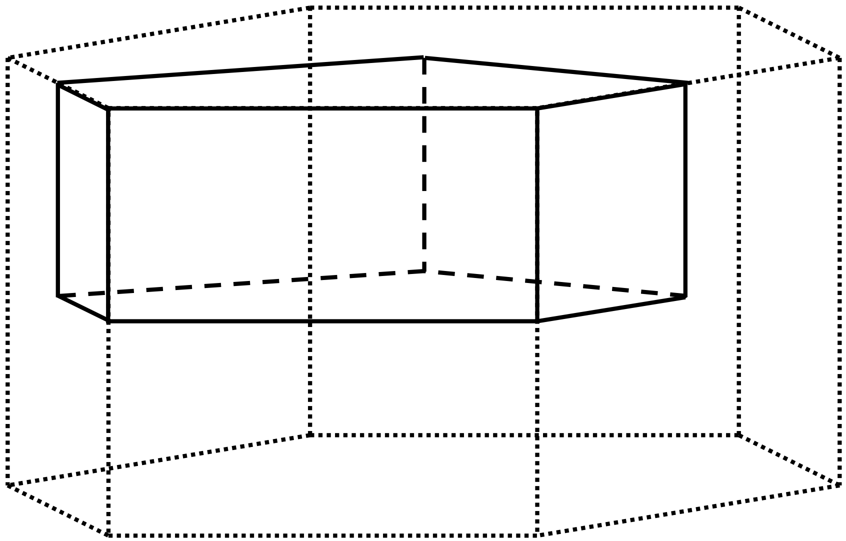
2. There are common symmetry operations

   Voronoï cell around I = 'large cell' 🕒 asymmetric domain

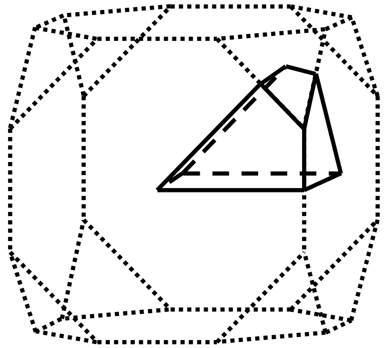
   There are equivalent points within the large cell.

Asymmetric domains Rodrigues space

$$\left(D_3, D_3\right)$$

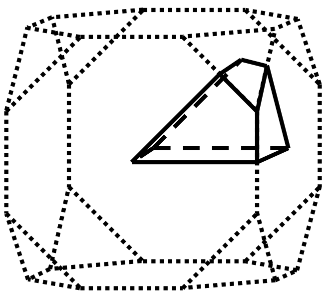


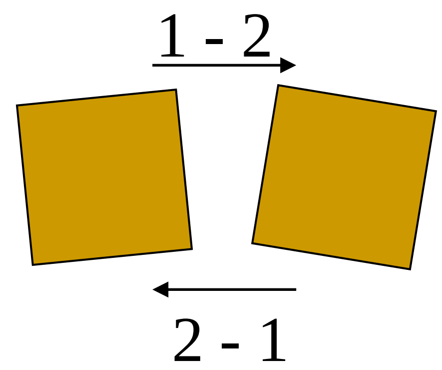
$$\left(O, O\right)$$

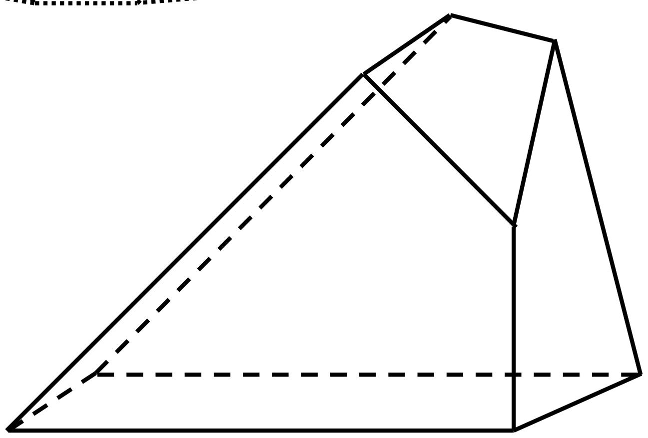


Asymmetric domains Rodrigues space

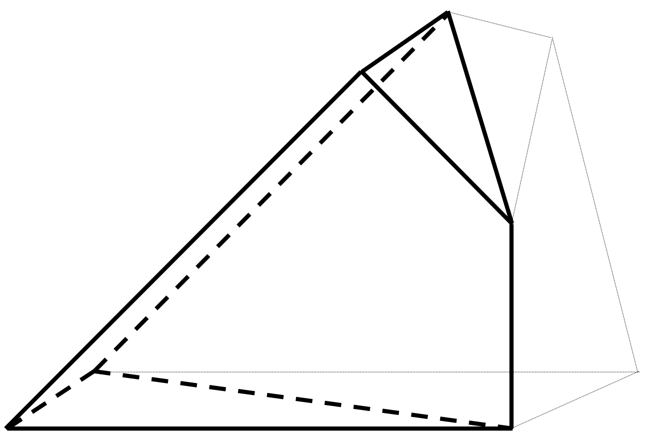
- additional equivalence
  for indistinguishible objects







(O,O)

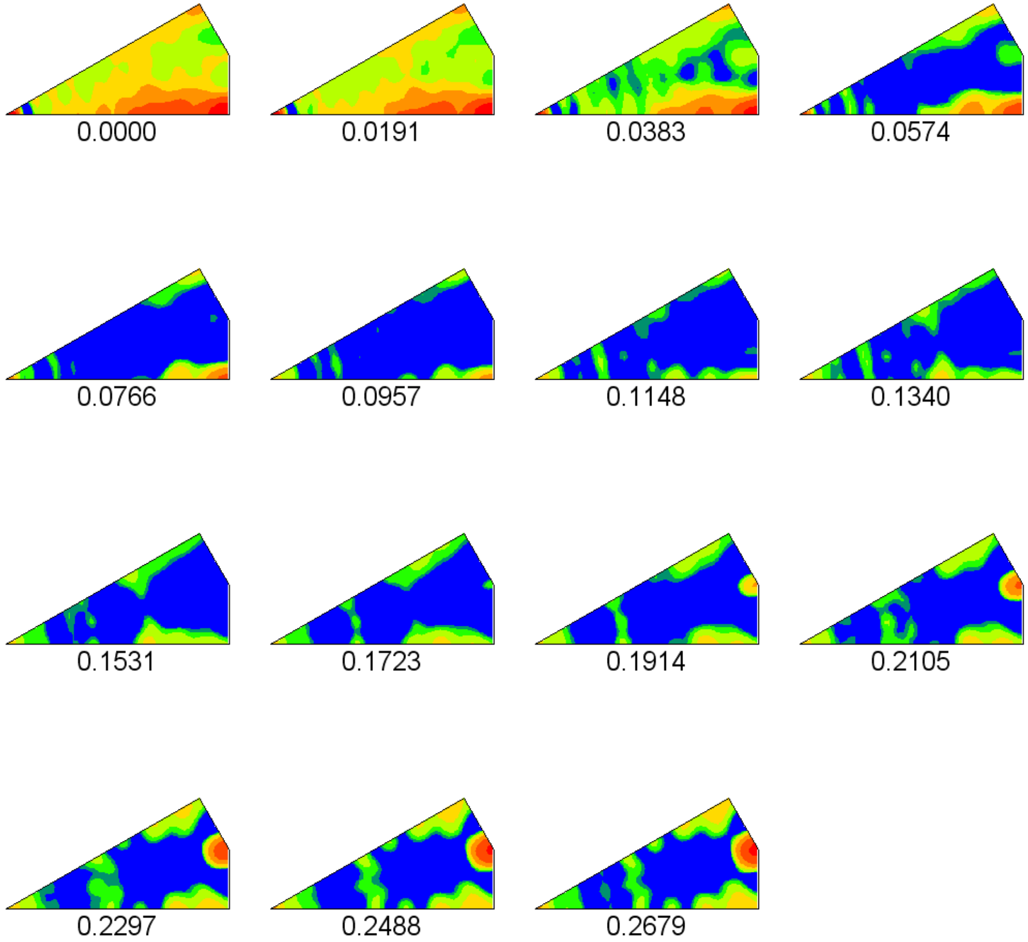


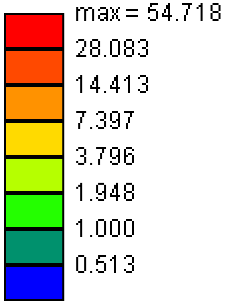
$(O,O)/2$

Asymmetric domains Rodrigues space

Extruded Ti-α

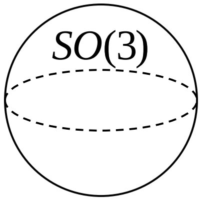
$$\left(D_6, D_6\right)$$



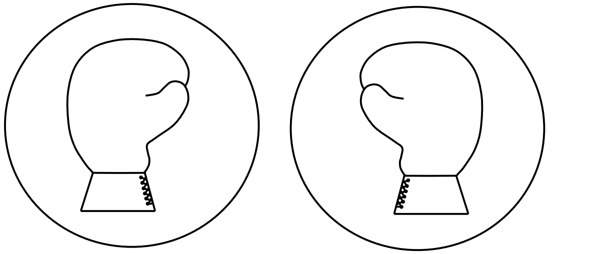


Asymmetric domains

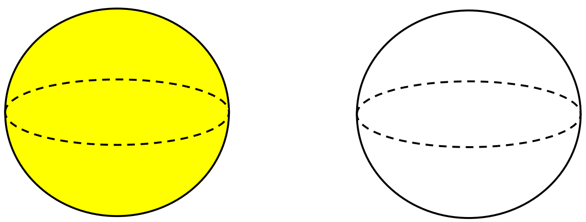
Previous considerations:
proper rotations and proper symmetry operations



Standard approach in textures:
enatiomorphic crystals – different phases

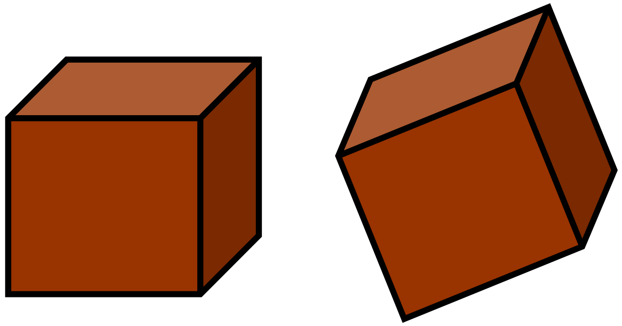


Proper rotations Improper rotations



$$O(3) = SO(3) \cup \textit{second component}$$

Misorientation angle distribution



[2 1 0], 131.81deg
= [1 1 1], 60.00deg

Mis(dis)orientation –*you must be disoriented*

Disorientation angle - the smallest of angles of all rotations leading from one orientation to the other

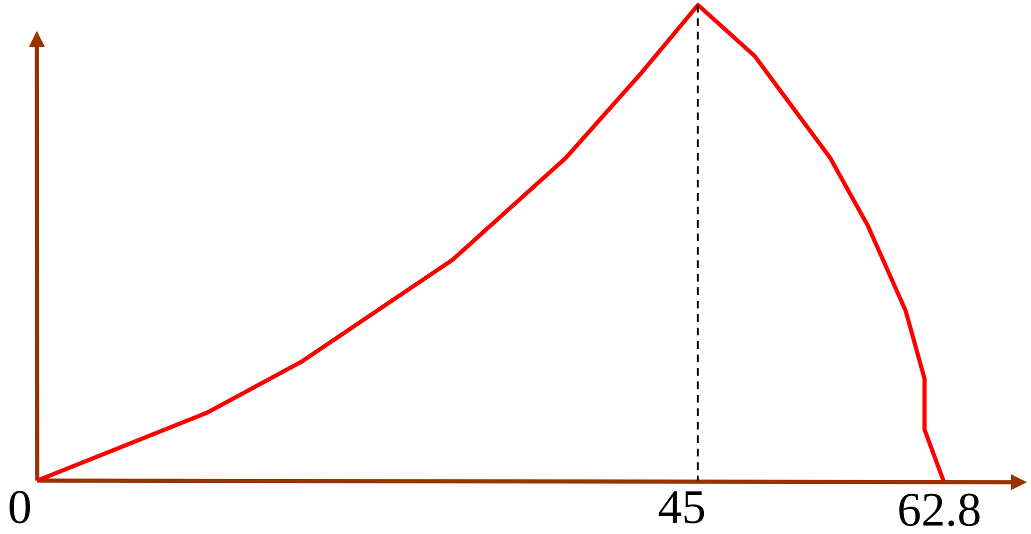
Question: what is the frequency of occurence of these smallest angles when the crystalites are randomly distributed?

Reference distribution

Misorientation angle distribution

The case of (O,O)

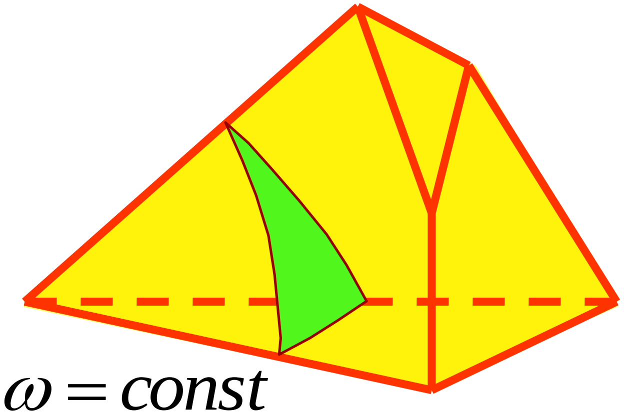
Mackenzie, 1958, Handscomb, 1958

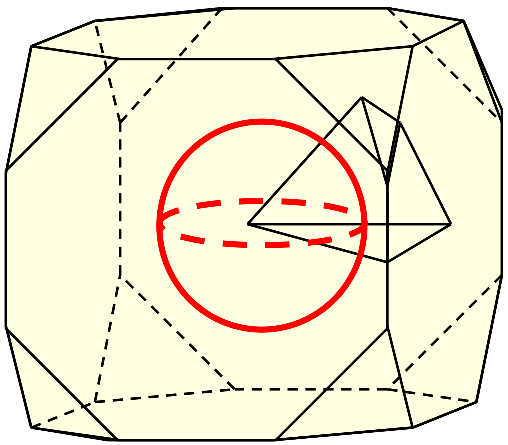


Mackenzie distribution

Misorientation angle distribution

The frequency of occurence of misorientation angles is related to the area of the surface ω=const in the asymmetric domain (based on the smallest angles)



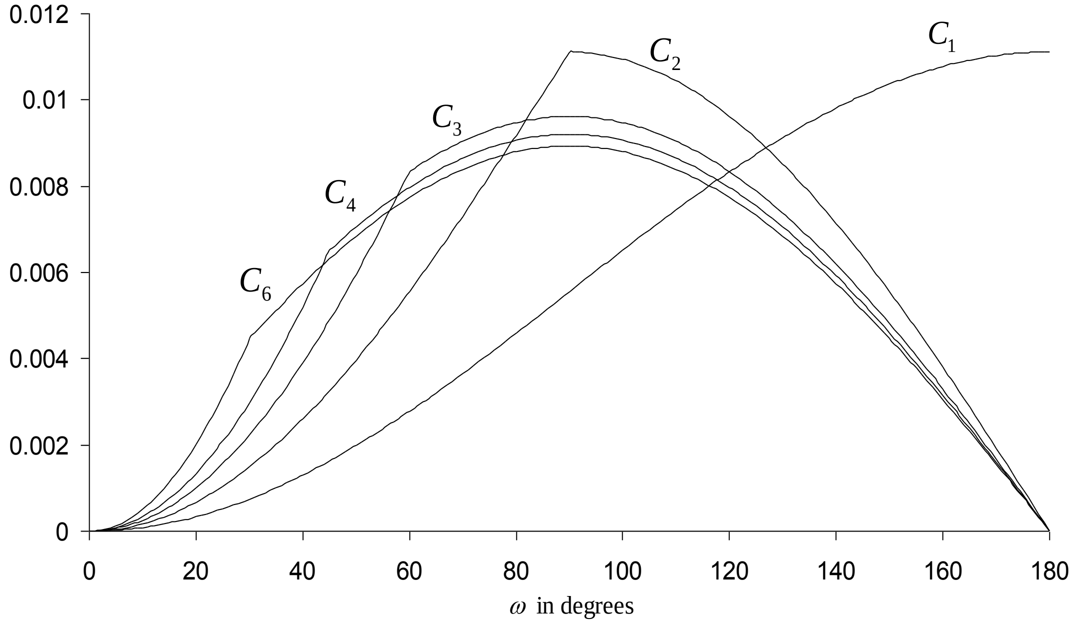


invariant volume (density of random orientations)
+ shape of the large cell

misorientation angle distribution

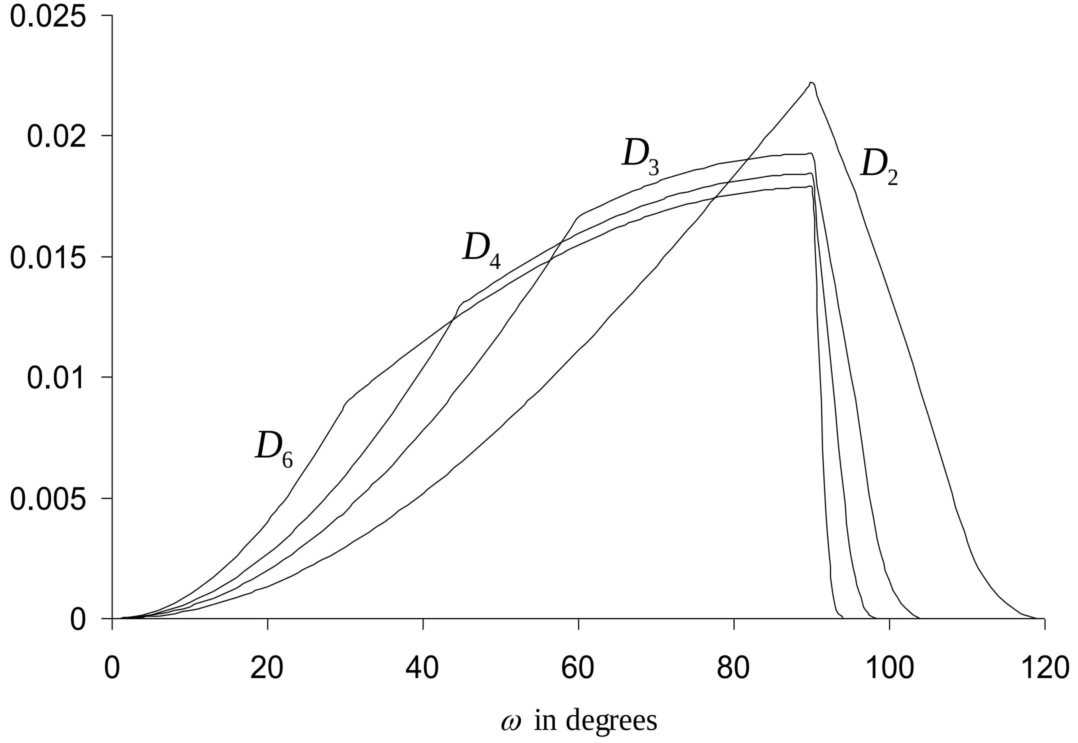
Misorientation angle distribution

Cyclic symmetries

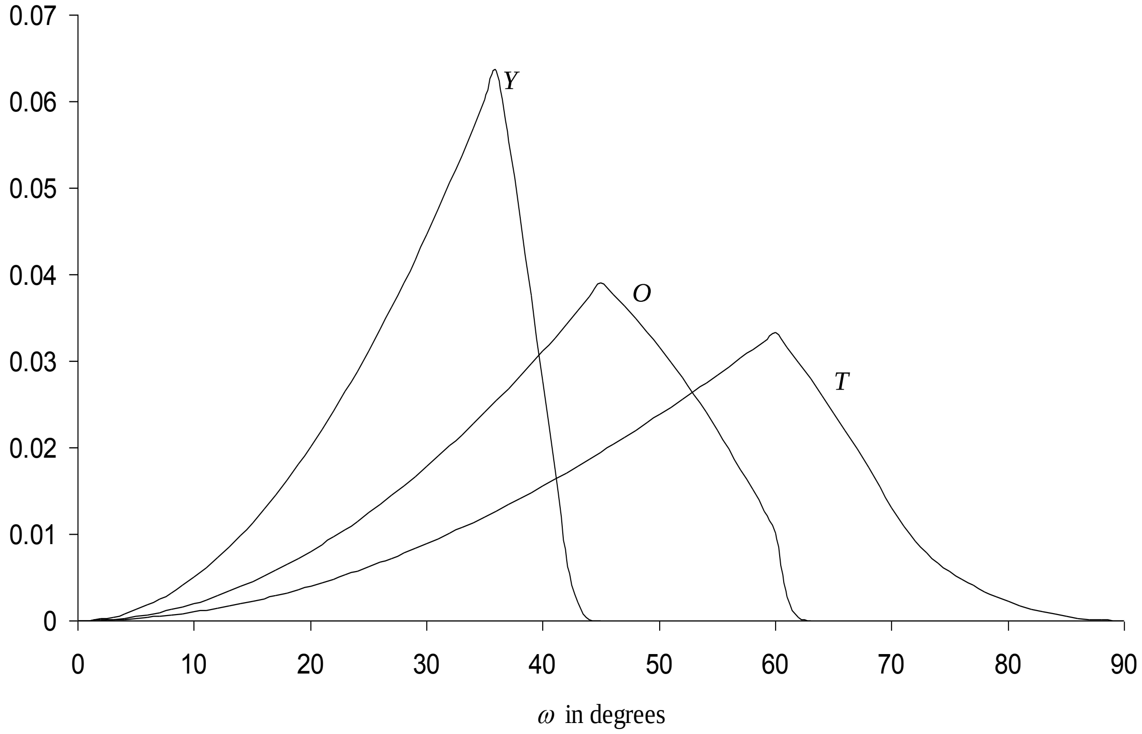


Misorientation angle distribution

Dihedral symmetries



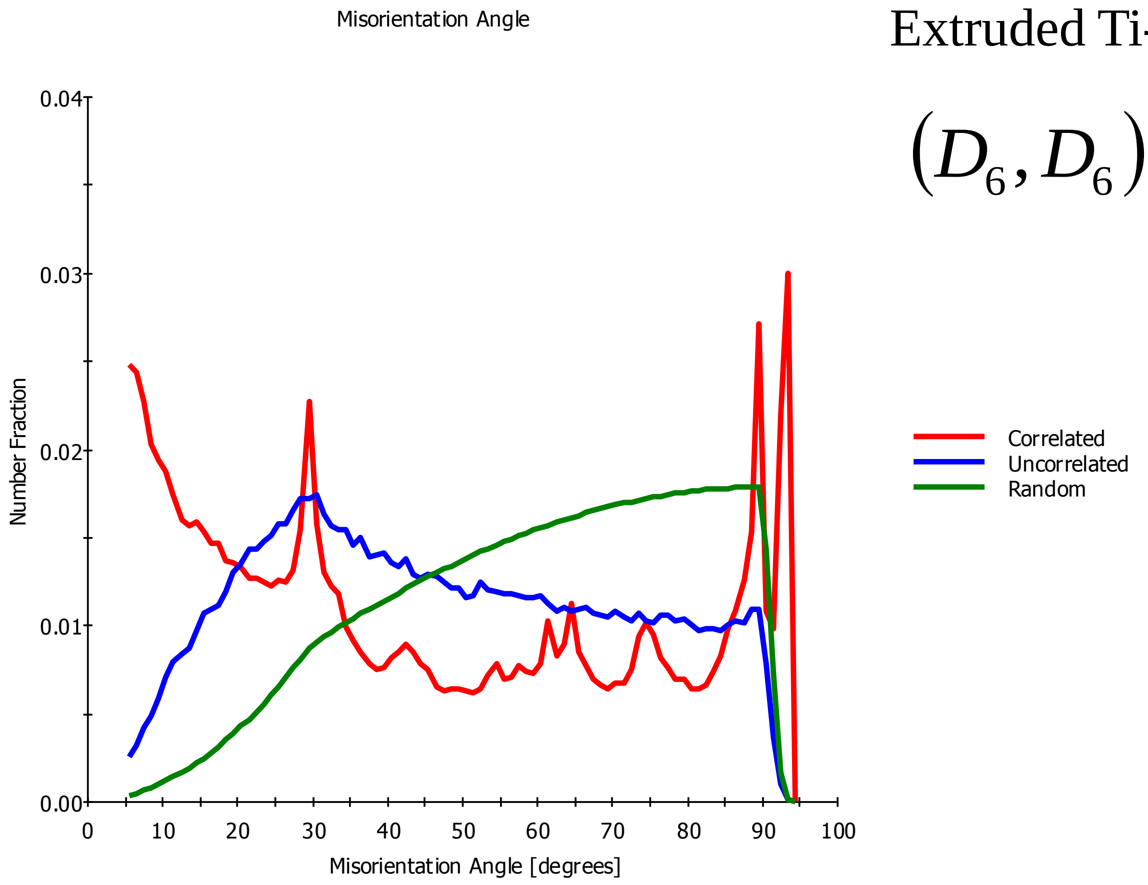
Misorientation angle distribution



Misorientation angle distribution

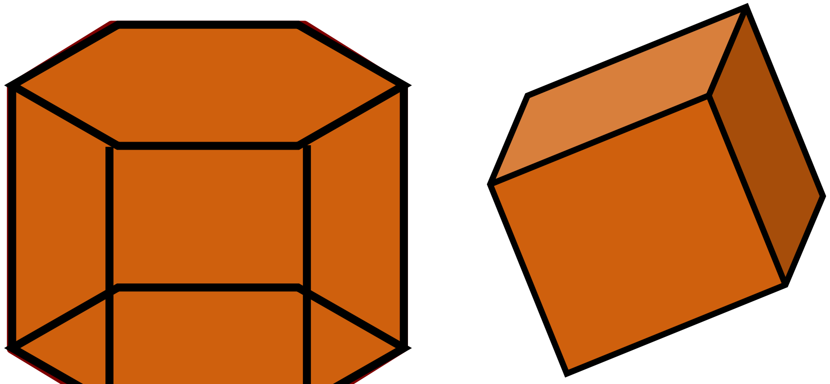
Extruded Ti-α

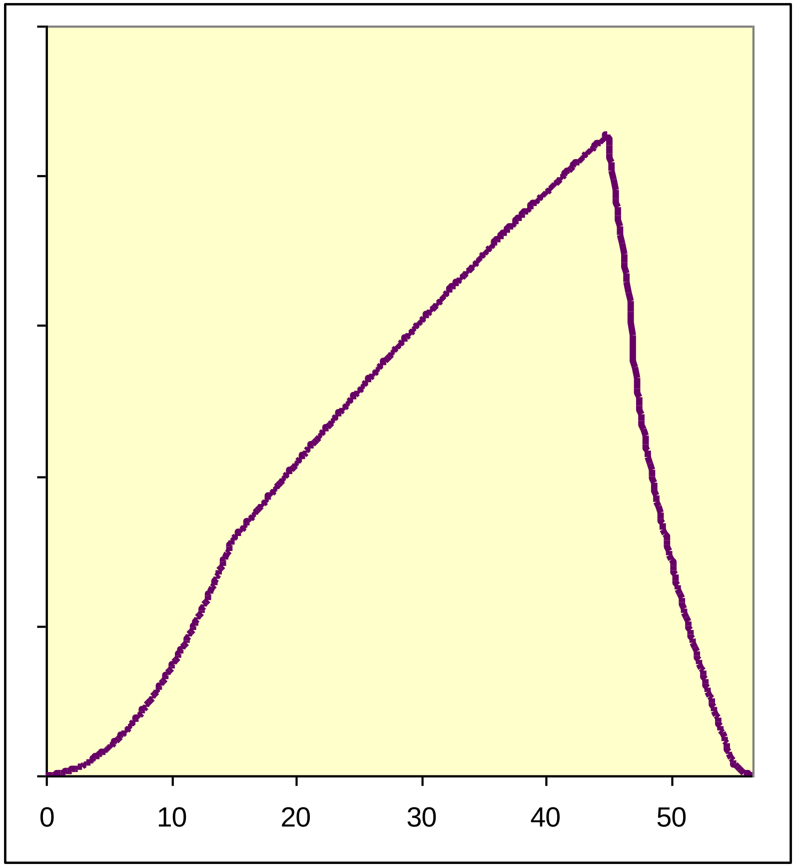
$$\left(D_6, D_6\right)$$



Misorientation angle distribution

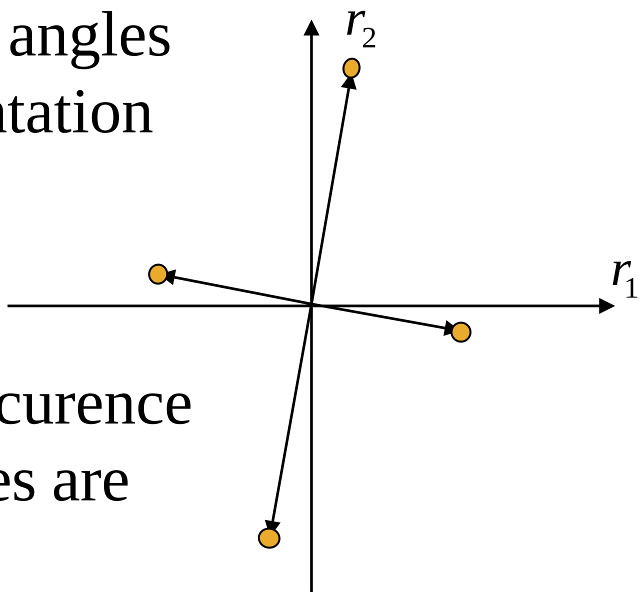
Multi-phase cases





Misorientation angle distribution

Axis corresponding to the smallest of angles of all rotations leading from one orientation to the other.



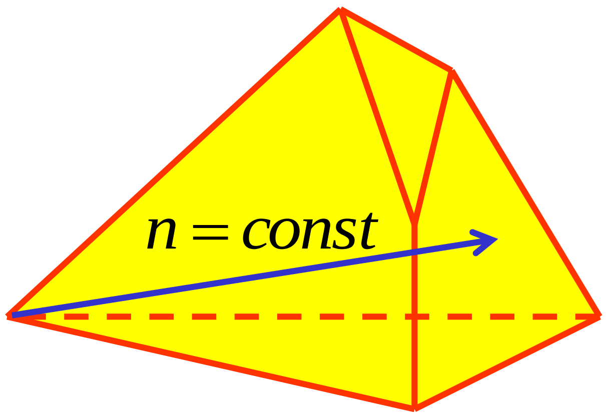
Question: what is the frequency of occurence of these these axes when the crystalites are randomly distributed?

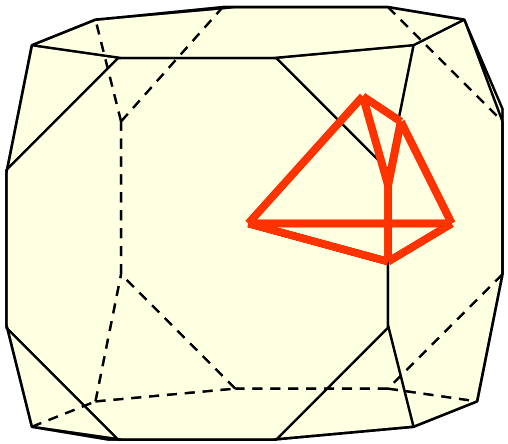
Reference distribution

The cubic case – Mackenzie, 1964

Misorientation axis distribution

In the Rodrigues space, the distance of the planes bounding the asymmetric domain is related to the frequency of occurence of misorientation axes.





invariant volume (density of random orientations)
+ shape of the large cell

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misorientation axis distribution

Misorientation axis distributions

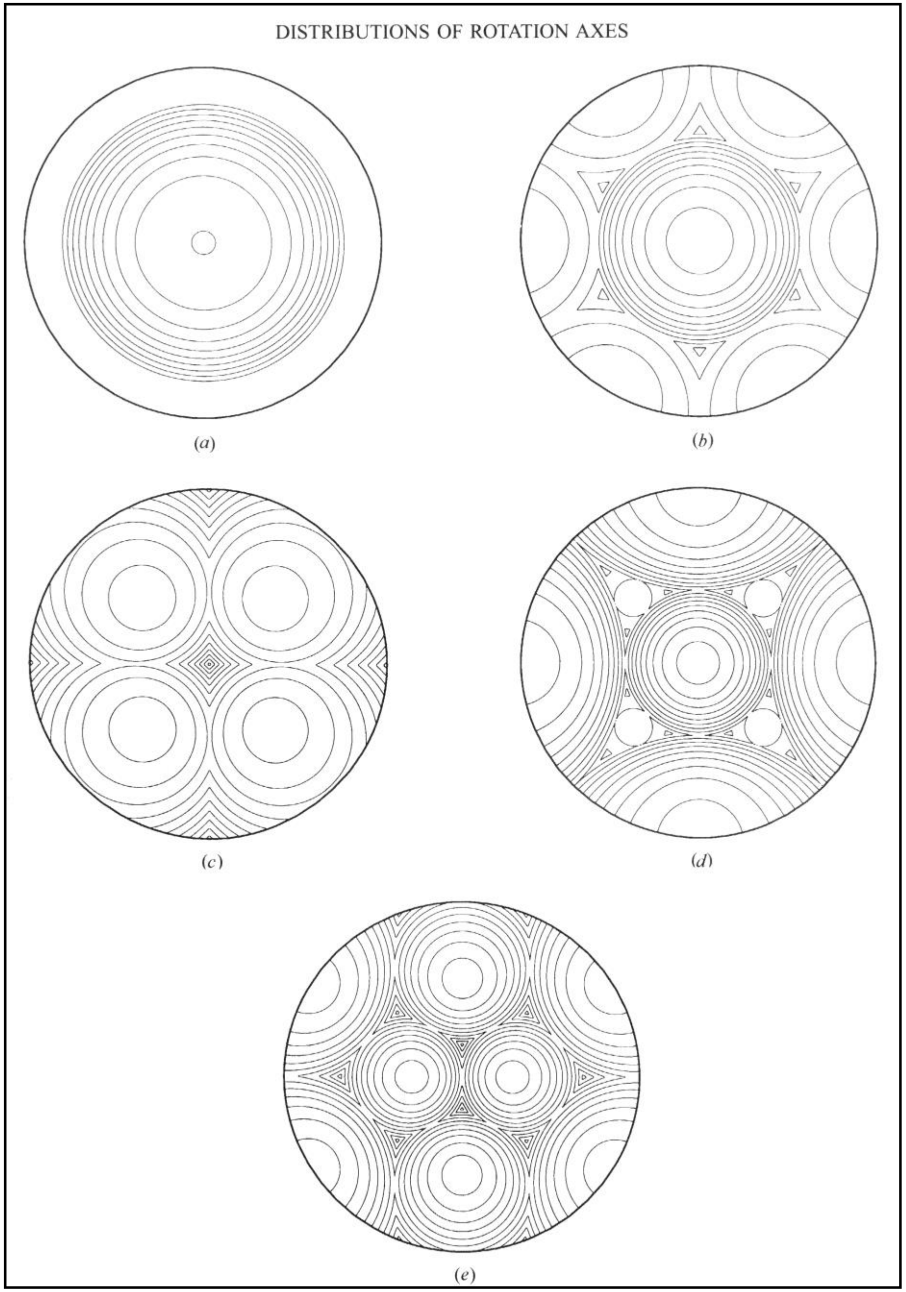
$a - C_3$

$b - D_3$

$c - T$

$d - O$

$e - Y$



CSL misorientations

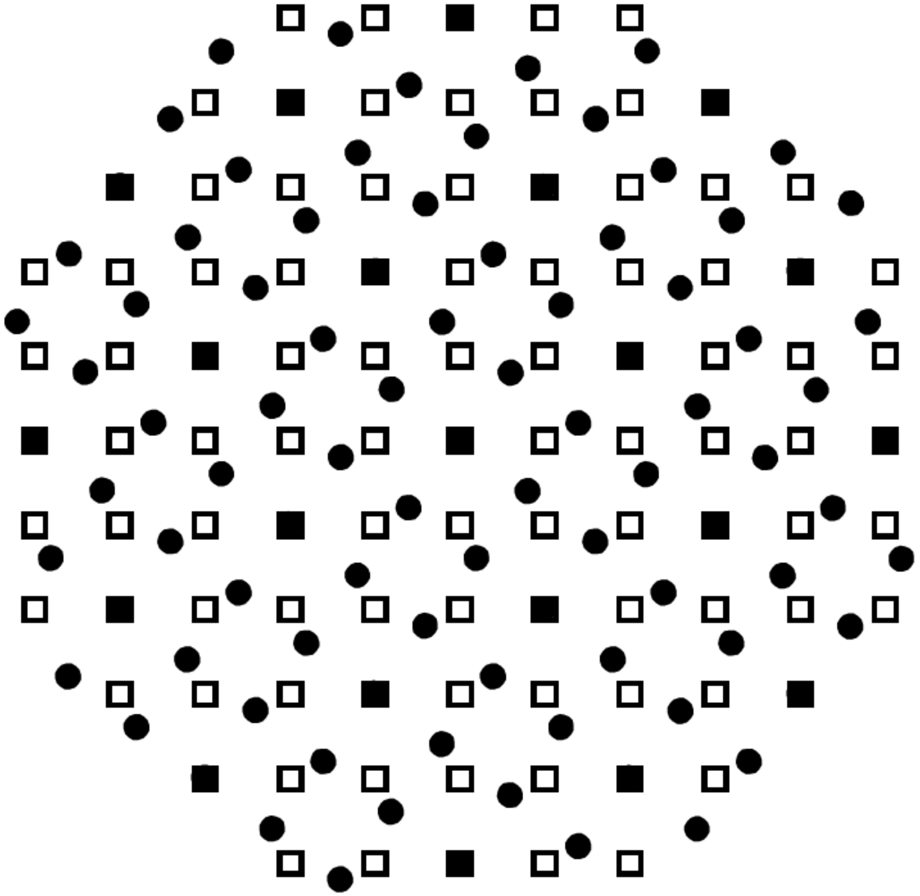
Coincident lattices

G.Friedel, (1926).

Kronberg, M. L. and F. H. Wilson (1949), *Trans. Met. Soc. AIME*, **185**, 501 (1947).

Coincident *Site* Lattice

Σ - reciprocal of the fraction of overlapping lattice nodes.



36.8699° <100>

CSL misorientations

cub

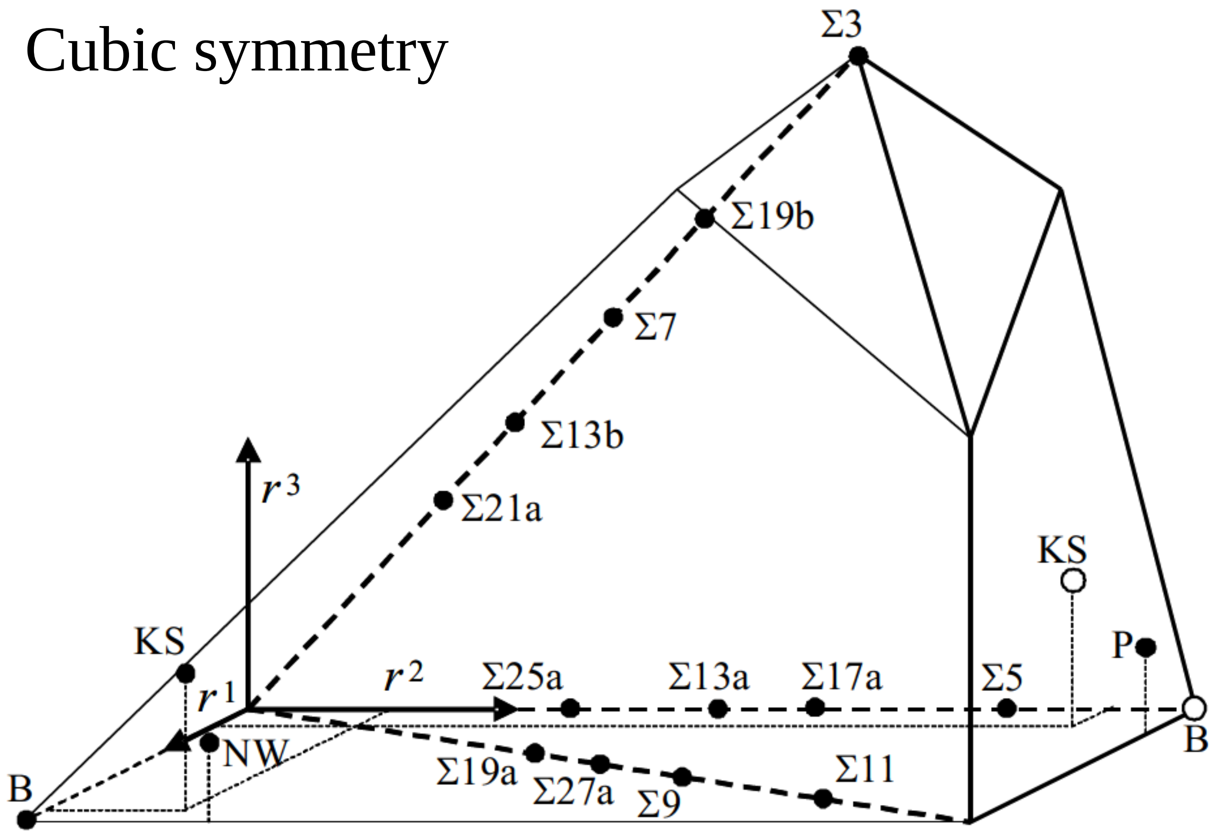
Σ	*Angle*	*Axis*
1	0.0000	
3	60.0000	<111>
5	36.8699	<100>
7	38.2132	<111>
9	38.9424	<110>
11	50.4788	<110>
13a	22.6199	<100>
13b	27.7958	<111>
15	48.1897	<210>
17a	28.0725	<100>
17b	61.9275	<221>
19a	26.5254	<110>
19b	46.8264	<111>
21a	21.7868	<111>
21b	44.4153	<211>
23	40.4591	<311>
25a	16.2602	<100>
25b	51.6839	<331>
27a	31.5863	<110>
27b	35.4309	<210>

hcp

Σ	*Angle*	*Miller indices of axis*
7	21.7868	<0 0 1>
10	78.4630	<2 1 0>
11	62.9643	<2 1 0>
13	27.7958	<0 0 1>
14	44.4153	<2 1 0>
17	86.6277	<1 0 0>
18	70.5288	<1 0 0>
19	13.1736	<0 0 1>
22	50.4788	<1 0 0>
25	23.0739	<2 1 0>
26	87.7958	<8 0 1>
27	38.9424	<1 0 0>
29	66.6372	<16 0 3>
31a	17.8966	<0 0 1>
31b	56.7436	<5 1 0>
34	53.9681	<4 0 1>
35a	34.0477	<2 1 0>
35b	57.1217	<2 1 0>
37a	9.4300	<0 0 1>
37b	72.7047	<7 2 0>

CSL misorientations and ORs

Cubic symmetry



Summary

Orientation analysis is influenced by symmetries of objects

Crystal symmetry and statistical sample symmetry

Asymmetric domains:

- Euler angles – nice for low symmetries
- Rodrigues parameterization – Voronoï tessellation

Reference misorientation angle/axis distributions