Workshop on Mathematical Crystallography
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Introduction to the crystallography of twins

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Point space vs. Vector space in crystallography

- Point space is the ordinary affine space (direct space, crystal space). It has an origin and N basis vectors, N being the dimensions of the space. Atoms “live” in point space.
- Vector space is an abstract vector space whose elements are vectors. It has no origin but in it the zero vector is defined. When “decorated” with an $Å^{-1}$ metric, it gives the reciprocal space.
- Obviously, point space and vector space are dual.

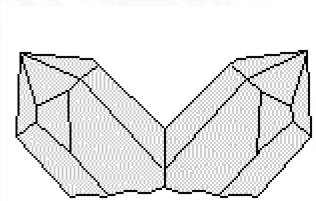
What is a twin?

With space group

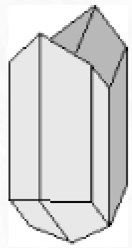
No space group

A twin is a heterogeneous edifice built by homogeneous crystals (individuals) of the same phase in different orientations, related by an operation (the twin operation) that does not belong to the point group of the individual.

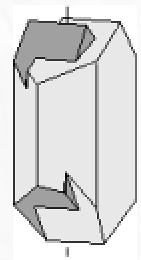
Mapping of individuals in twins



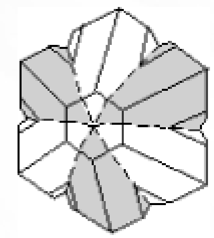
Reflection in $\{11\bar{2}2\}$



Reflection in (100)



Rotation about [001]



Reflection in {031} (cyclic twin)

Symmetry of a twin

- H_i is the point group of the i-th individual (same *type* for all the individuals)
- H* is the intersection group: $H^* = \cap_i H_i$.
- $\tilde{t}$ is a twin operation
- K is the (chromatic) point group obtained as extension of H* by $\tilde{t}$
- The coset decomposition of K in terms of H* gives N = |K|/|H*| cosets (twin laws), from each of which one coset representative (twin operation) is chosen.

|K| is the order of K

Twin operation, twin element, twin law

- **Twin operation**: the isometry mapping the orientation of one individual onto the orientation of another individual.
- **Twin element**: the geometrical element in *direct space* (plane, axis, center) about which the twin operation is performed.
  - Correspondingly, twins are classified as reflection twins, rotation twins and inversion twins
- Twin law: the set of twin operations equivalent under the point group of the individual, obtained by coset decomposition.

Genetic classification of twins – 1 – Transformation twins

- Transformation twins form when a phase transition occurs where the parent and daughter phase are in group-subgroup ($G \rightarrow H$) relation.
- The twin law(s) is(are) the coset(s) obtained by decomposing G in terms of H.
- The twin point group (chromatic point group) K is isomorphic to G: the twin and the individual are in group-subgroup relation.
- The driving force is the crossing of the free energy of the two phases at the transition temperature.
- The twin forms because the transition occurs at the solid state (no recrystallization), within a constant volume (we make abstraction of the thermal expansion/contraction).

Genetic classification of twins – 2 – Mechanical twins

- Mechanical twins occur where a physical action (oriented pressure) is applied on the crystal.
- The formation mechanism of the twin consists in a glide of atomic planes along a direction resulting from the physical action applied on the crystal and the low(er)-energy bonding directions within the crystal.
- In general, there is no group-subgroup relation between the twin point group and the individual point group.
- If the crystal structure does not have low(er)-energy bonding directions, the twin does not form: cleavage or fracture may instead result.

Genetic classification of twins – 3 – Growth twins

- A growth twin is an "accident": a single, untwinned crystal is more stable.
- In general, there is no group-subgroup relation between the twin point group and the individual point group.
- The twin may form at the nucleation stage, at the growth stage, or as oriented attachment of grown crystals.
- In order for a twin to form, a structural continuity must exist across the interface.
- When the oriented attachment mechanism is responsible for the formation of a twin, the interface coincides with a developed face of the crystal.
- How and why a crystal will or will not form a growth twin?

Lattice restoration vs. structure restoration

- The lattice represents the periodicity of the crystal structure.
- A high degree of lattice restoration is a necessary, although not sufficient, condition for a good structural match across the interface.
- The lattice restoration is measured by the twin index ***n*** (inverse of the fraction of the lattice nodes restored by the twin operation) and by the obliquity **ω** (deviation from perfect restoration).

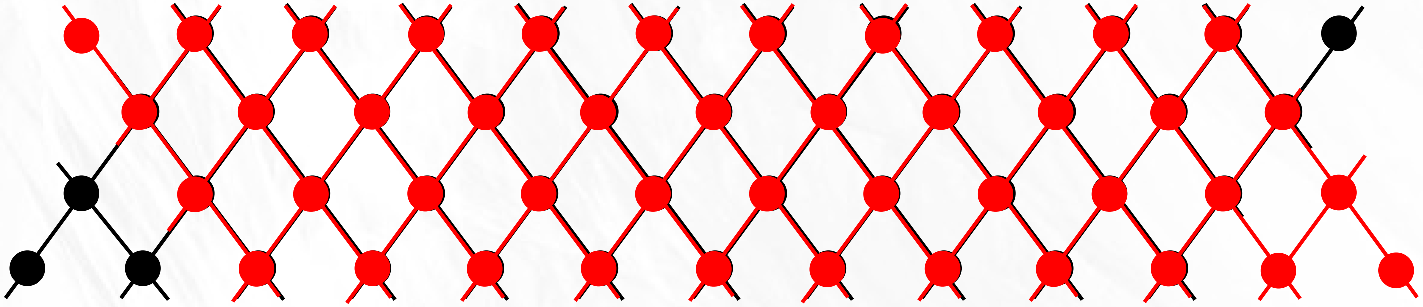
Twin lattice and twin index

- The twin index is the number of lattice nodes restored ($\omega = 0$) or quasi-restored ($\omega \neq 0$) by the twin operation.
- The (quasi)-restored nodes define a lattice, the **twin lattice**.
- (Quasi)-restored nodes define the cell based on the pair of elements (plane/direction) defining the cell of the twin lattice.
- The twin lattice either coincides with the lattice of the individual (twinning by merohedry) or is a sublattice of it (twinning be reticular merohedry/polyholohedry).

Categories of twins: lattice quasi-restoration and symmetry of the twin lattice

Hereafter K is the achromatic point group isomorphic to the chromatic twin point group

Twinning by merohedry



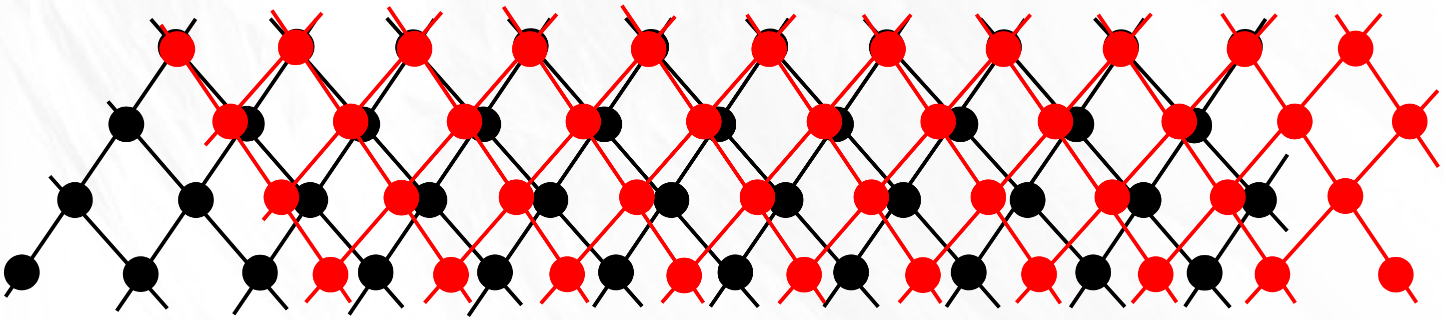
All nodes are restored by the twin operation: we say that **the twin index is *n* = 1**

H* = H; K ⊃ H

Subclassificaton of twinning by merohedry

- H = point group of the individual
- D = holohedral point group of the individual
- D($\mathbf{L}_{ind}$) = point group of the lattice of the individual
- D($\mathbf{L}_{T}$) = point group of the lattice of the twin
- If D($\mathbf{L}_{ind}$) > D the individual has a specialized metric
- If $\tilde{t} \in$ D, we speak of **syngonic merohedry**
- If $\tilde{t} \in$ D($\mathbf{L}_{ind}$) but t $\notin$ D, we speak of **metric merohedry**

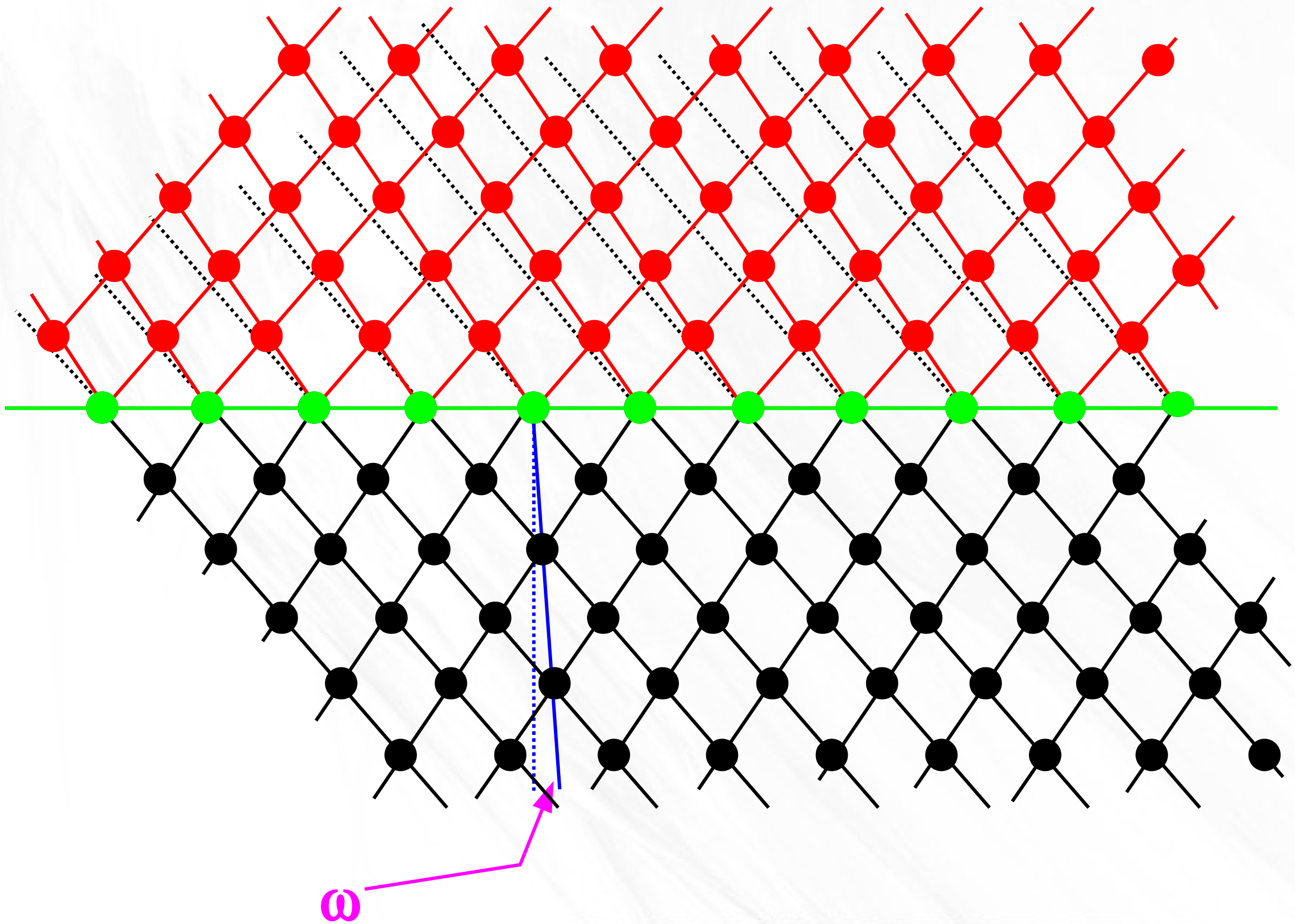
Twinning by pseudo-merohedry



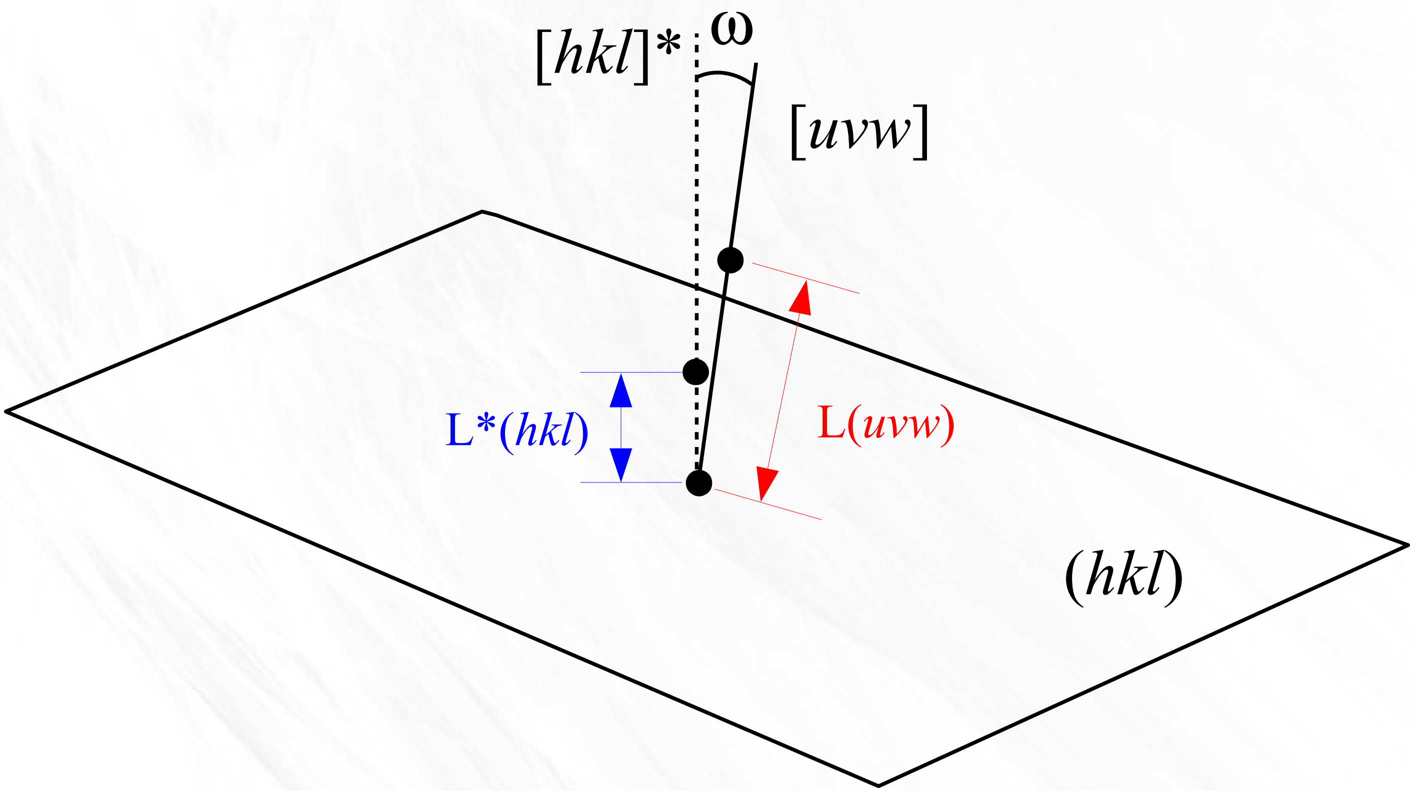
All nodes are *quasi*-restored by the twin operation: we say that **the twin index is n = 1**

$$H^* = H_{(\omega = 0)};\ K \supset H$$

Definition of obliquity



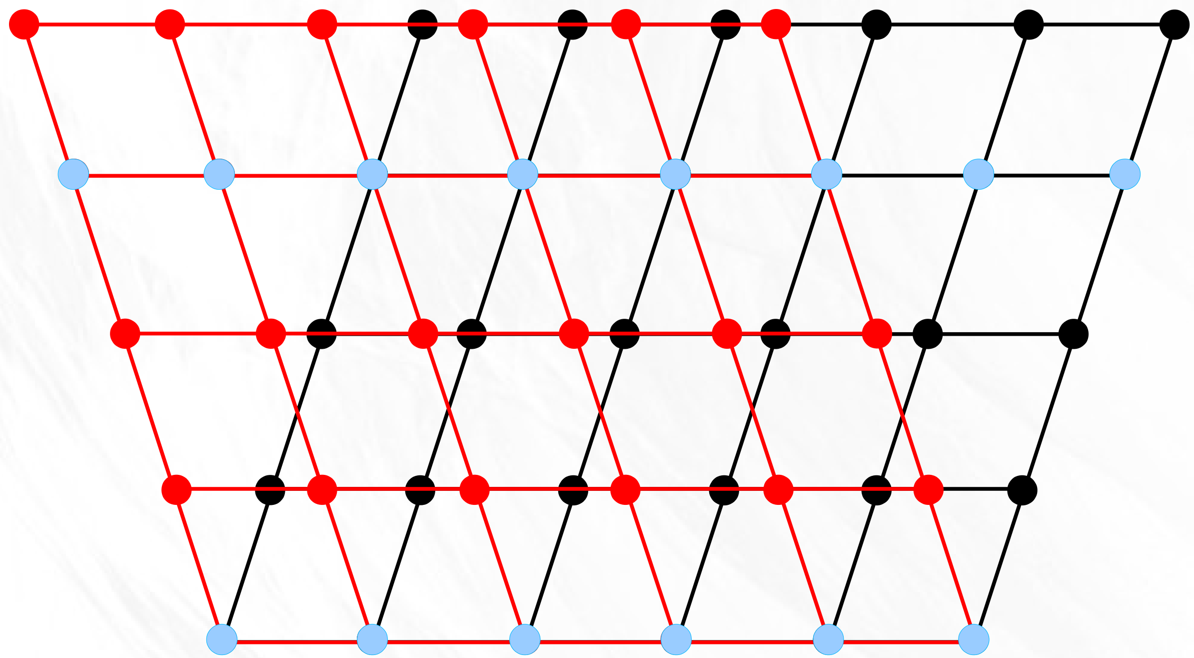
Computation of the obliquity



$$L^*(hkl)L(uvw)\cos\omega = \langle hkl|\boldsymbol{a}^*\boldsymbol{b}^*\boldsymbol{c}^*\rangle\langle \boldsymbol{abc}|uvw\rangle = |hu+kv+lw|$$

$$\omega = \cos^{-1}|hu+kv+lw|/L^*(hkl)L(uvw)$$

Twinning by reticular merohedry

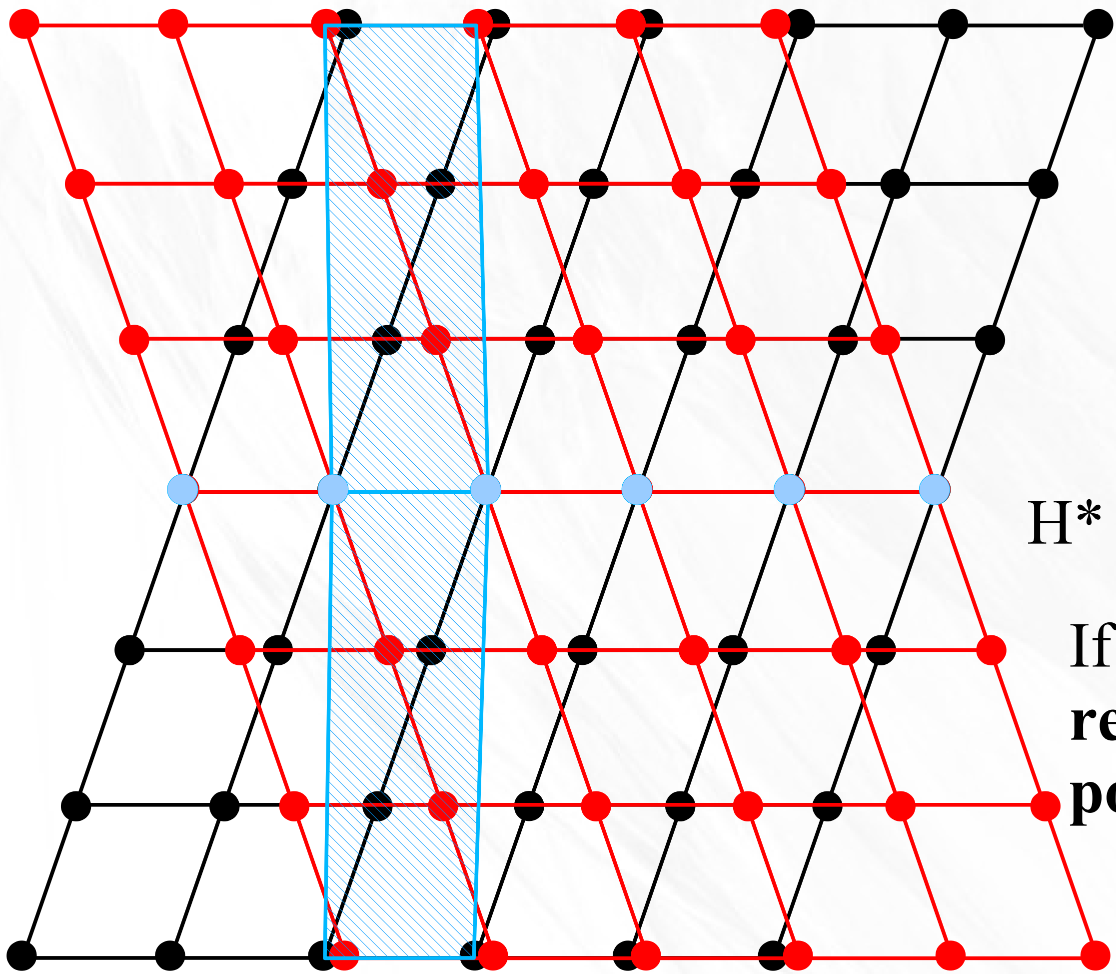


One node out of three is restored by the twin operation: we say that **the twin index is *n* = 3**

H* ≠ H; K ⊃ H*

If K = H we speak of **reticular polyholohedry**

Twinning by reticular pseudo-merohedry



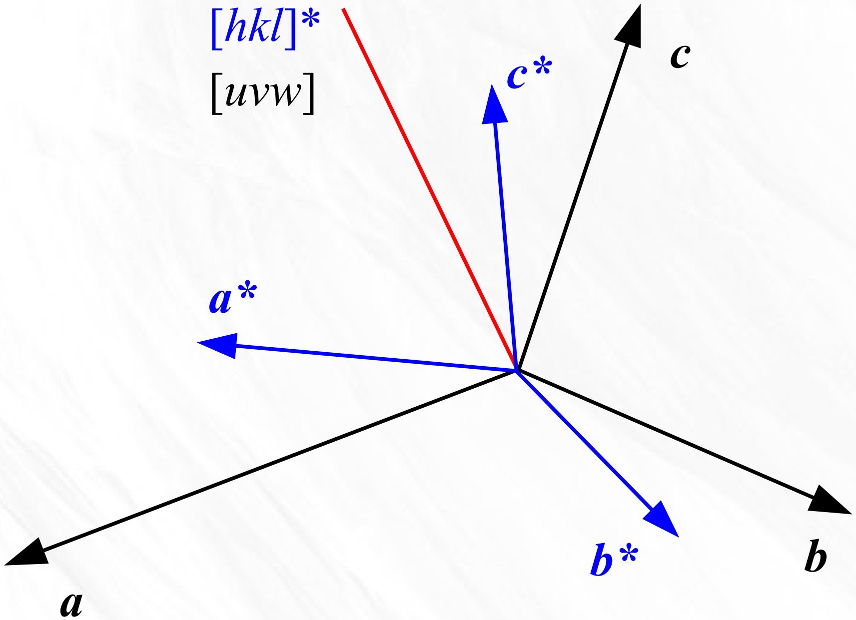
One node out of three is *quasi*-restored by the twin operation: we say that **the twin index is *n* = 3**

$H^* \neq H_{(\omega = 0)}$; $K \supset H^*$

If K = H we speak of **reticular pseudo-polyholohedry**

How to find the direction [uvw] quasi-perpendicular to (hkl)?

Easy! Find the irrational expression of [*hkl*]* in direct space



How?

Easy!

Find u,v,w (in general non-integer) satisfying:

$$\langle hkl|\boldsymbol{a}^*\boldsymbol{b}^*\boldsymbol{c}^*\rangle = \langle uvw|\boldsymbol{abc}\rangle$$

$$\langle hkl|\mathbf{I}|\boldsymbol{a}^*\boldsymbol{b}^*\boldsymbol{c}^*\rangle = \langle uvw|\boldsymbol{abc}\rangle$$

$$\langle hkl|\mathbf{G}^*\mathbf{G}|\boldsymbol{a}^*\boldsymbol{b}^*\boldsymbol{c}^*\rangle = \langle uvw|\boldsymbol{abc}\rangle$$

$$\langle hkl|\mathbf{G}^*|\boldsymbol{abc}\rangle\langle\boldsymbol{abc}|\boldsymbol{a}^*\boldsymbol{b}^*\boldsymbol{c}^*\rangle = \langle uvw|\boldsymbol{abc}\rangle$$

$$\langle hkl|\mathbf{G}^*|\boldsymbol{abc}\rangle 3 = \langle uvw|\boldsymbol{abc}\rangle$$

$$\langle hkl|\mathbf{G}^* = \langle uvw|$$

and of course... $\langle uvw|\mathbf{G} = \langle hkl|$

Exercise

Celestine, $SrSO_4$, *Pbnm* $a = 8.359$Å, $b = 5.352$Å, $c = 6.866$Å,

Twinned on (210)
Find the directions quasi-perpendicular to (210) and CHOOSE ONE!

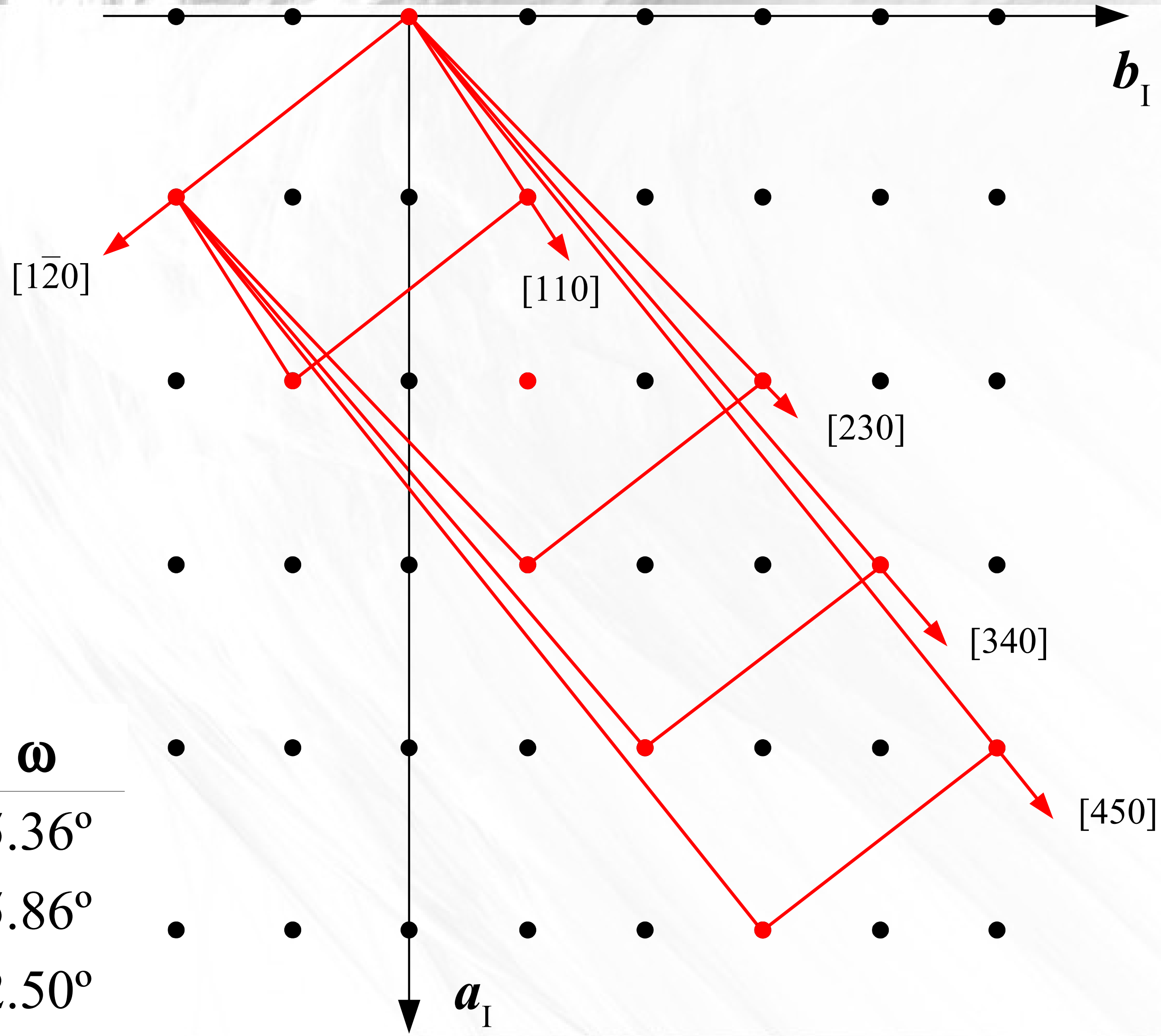
$$\langle 210| \begin{vmatrix} 1/a^2 & 0 & 0 \\ 0 & 1/b^2 & 0 \\ 0 & 0 & 1/c^2 \end{vmatrix} = \langle 0.02862 \quad 0.03491 \quad 0| = \langle 1 \quad 1.220 \quad 0|$$

u	*v*	*v/u*
1	1	1
1	2	2
2	3	1.5
3	4	1.333
4	5	1.25

Calculate the obliquity

$$\omega = \cos^{-1}|hu+kv+lw|/L^*(hkl)L(uvw) = \cos^{-1}\frac{\langle hkl|uvw\rangle}{\sqrt{\langle hkl|\mathbf{G}^*|hkl\rangle}\sqrt{\langle uhv|\mathbf{G}|uvw\rangle}}$$

uvw	**ω**
110	5.36º
120	14.03º
230	5.86º
340	2.50º
450	0.69º



uvw	ω
110	5.36°
230	5.86°
340	2.50°
450	0.69°

Summary

uvw	ω	*n*
110	5.36º	3
230	5.86º	7
340	2.50º	5
450	0.69º	13

Cell parameters of the twin lattice

A matter of basis transformation....

$$\langle \mathbf{a} \quad \mathbf{b} \quad \mathbf{c} | \mathbf{P} = \langle \mathbf{a}' \quad \mathbf{b}' \quad \mathbf{c}' |$$

$$\mathbf{G}' = | \mathbf{a}' \quad \mathbf{b}' \quad \mathbf{c}' \rangle \langle \mathbf{a}' \quad \mathbf{b}' \quad \mathbf{c}' | =$$

$$= \mathbf{P}^t | \mathbf{a} \quad \mathbf{b} \quad \mathbf{c} \rangle \langle \mathbf{a} \quad \mathbf{b} \quad \mathbf{c} | \mathbf{P} = \mathbf{P}^t \mathbf{G} \mathbf{P}$$

$$\mathbf{P} = \begin{vmatrix} u_{1,hkl} & u_{2,hkl} & u_{\perp} \\ v_{1,hkl} & v_{2,hkl} & v_{\perp} \\ w_{1,hkl} & w_{2,hkl} & w_{\perp} \end{vmatrix}$$

But check the determinant!

$[u_{1,hkl}v_{1,hkl}w_{1,hkl}]$ and $[u_{2,hkl}v_{2,hkl}w_{2,hkl}]$ are contained in (*hkl*)
(choose the shortest!)

$[u_{\perp}v_{\perp}w_{\perp}]$ is the direction quasi-perpendicular to (*hkl*)

Directions [uvw] contained in a plane (hkl)

A plane of the family (*hkl*) which passes through the origin is $hx+ky+lz = 0$.

A direction [*uvw*] passes through the origin and the node *uvw*.

The direction [*uvw*] is contained in the plane (*hkl*) if $hu+kv+lw = 0$.

Calculate the cell parameters of the (210) twin in celestine.

Cell parameters of the (210) twin in celestine

$$[u_{1,hkl}v_{1,hkl}w_{1,hkl}] = [001]$$
$$[u_{2,hkl}v_{2,hkl}w_{2,hkl}]\ [1\bar{2}0]$$
$$[u_{\perp}v_{\perp}w_{\perp}]=[340]$$

$$\mathbf{P} = \begin{vmatrix} 0 & 1 & 3 \\ 0 & \bar{2} & 4 \\ 1 & 0 & 0 \end{vmatrix} \qquad |\mathbf{P}| = 10 > 0$$

N.B. $n = 5$ but $|\mathbf{P}| = 10$. Why?

Cell parameters of the (210) twin in celestine

$$\mathbf{P}^t\mathbf{G}\mathbf{P} = \begin{vmatrix} 0 & 0 & 1 \\ 1 & \bar{2} & 0 \\ 3 & 4 & 0 \end{vmatrix} \begin{vmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{vmatrix} \begin{vmatrix} 0 & 1 & 3 \\ 0 & \bar{2} & 4 \\ 1 & 0 & 0 \end{vmatrix} =$$

$$= \begin{vmatrix} 0 & 0 & c^2 \\ a^2 & -2b^2 & 0 \\ 3a^2 & 4b^2 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 & 3 \\ 0 & \bar{2} & 4 \\ 1 & 0 & 0 \end{vmatrix} = \begin{vmatrix} c^2 & 0 & 0 \\ 0 & a^2 + 4b^2 & 3a^2 - 8b^2 \\ 0 & 3a^2 - 8b^2 & 9a^2 + 16b^2 \end{vmatrix}$$

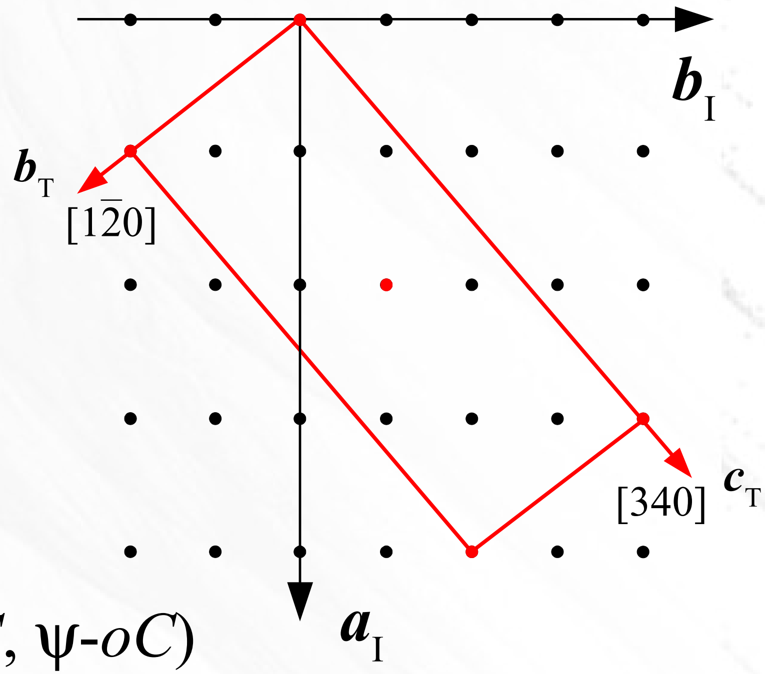
$$a_T = c_I = 6.866 \text{ Å} \qquad b_T = 13.581 \text{ Å} \qquad c_T = 32.972 \text{ Å}$$

$$\alpha_T = \cos^{-1}\frac{3a^2 - 8b^2}{b_T c_T} = \cos^{-1}\frac{-19.533}{13.581 \cdot 32.972} =$$

$$= \cos^{-1}(-0.0436) = 92.50$$

Twin lattice and pseudo-symmetry of (210) twin in celestine

a_T 6.866 Å; b_T = 13.581 Å:
c_T = 32.972 Å; α_T = 92.50º



mA, ψ-*oA* (easily transformed to *mC*, ψ-*oC*)

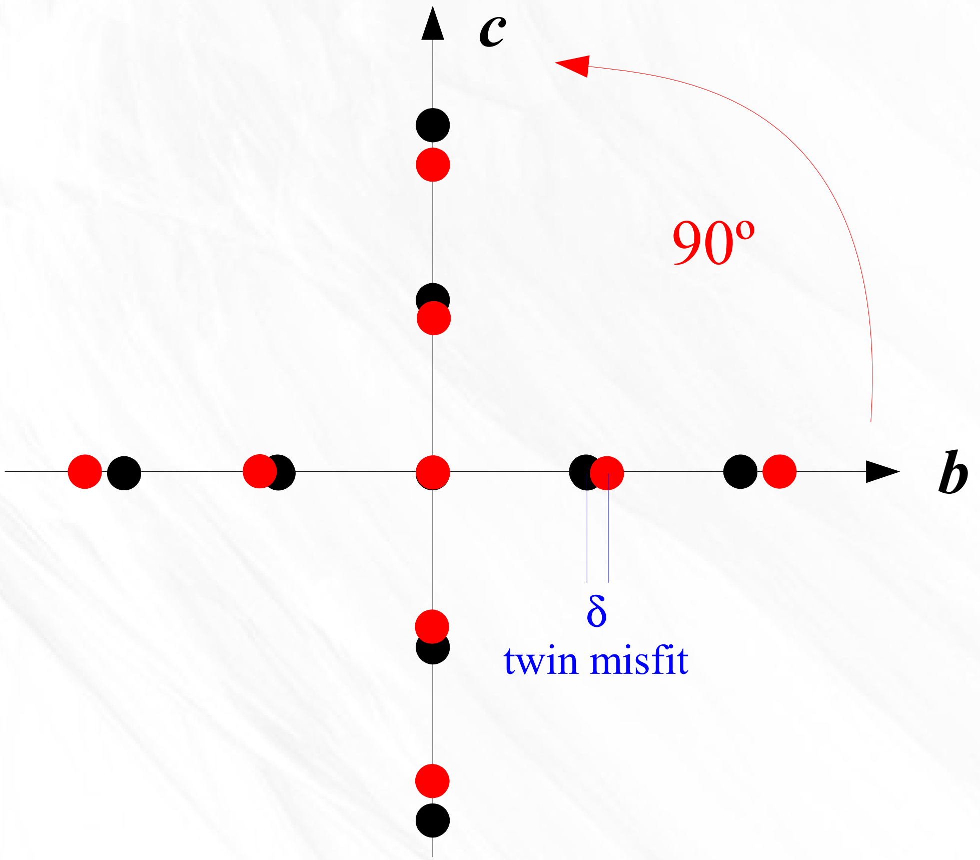
In twinning, the pseudo-symmetry is often more important than the true symmetry

TLS vs TLQS twinning

- Twin Lattice Symmetry (TLS): the restoration of the lattice of the individual (total or partial) is perfect.
- Twin Lattice Quasi-Symmetry (TLS): the restoration of the lattice of the individual (total or partial) is imperfect.
- TLQS only occurs when $\omega \neq 0$ if the twin operation is twofold.
- When the twin operation is a (direct or inverse) rotation of order higher than 2, TLQS may occur also for $\omega = 0$.

Zero-obliquity TLQS twinning

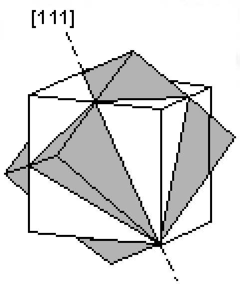
b ≈ ***c***



i-TLS vs. e-TLS

intrinsic **T**win **L**attice **S**ymmetry: when the perpendicularity (*hkl*)/[*uvw*] does not depend on the metric

Lattice system	lattice plane	lattice direction
triclinic	---	---
monoclinic (*b*-unique)	(010)	[010]
orthorhombic	(100) (010) (001)	[100] [010] [001]
tetragonal	(001) (*hkl*)	[001] [*hkl*]
rhombohedral and hexagonal (hexagonal axes)	(0001) (*hki*)	[001] [2*h*+*k*,*h*+2*k*,0]
Cubic	(*hkl*)	[*hkl*]



Rotation about ⟨111⟩

i-TLS vs. e-TLS

extrinsic **T**win **L**attice **S**ymmetry: when the perpendicularity (*hkl*)/[*uvw*] ***does*** depend on the metric

example: orthorhombic crystal with primitive lattice, pair (121)/[561]

a	*b*	*c*	ω(º)	type of twinning
4.00	5.000	8.00	2.85	TLQS
4.00	5.000	9.00	1.81	TLQS
4.00	5.200	9.00	0.36	TLQS
4.00	5.165	8.95	0	e-TLS

How to compute the twin index

A few preliminary definitions

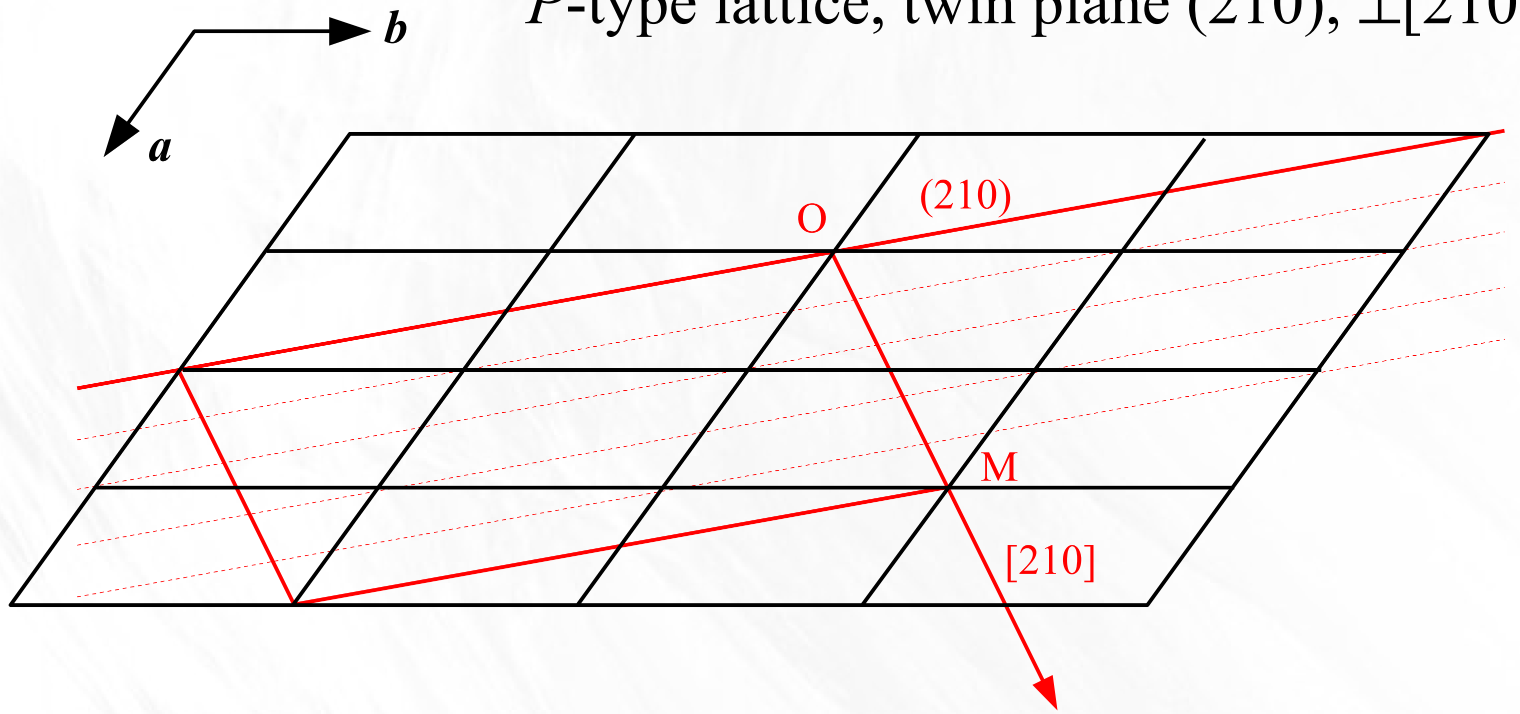
- **Twofold twins** are twins where only twin elements of order 2 exist (twofold twin axes, twin planes, twin inversion centers)
  - **First-degree twofold twins** or **binary twins** are twins where only one twin element of order 2 exists
  - **higher-degree twofold twins** are twins where more than one twin element of order 2 exist
- **Manifold twins** are twins where at least one twin element of order higher than 2 exists
  - **First-degree manifold twins** are twins where only one twin element of order higher than 2 exists
  - **higher-degree manifold twins** are twins where more than one twin element exist, of which at least one has order higher than 2

Twin index for twofold twins

A few preliminary definitions (continued)

(hkl) and [uvw] are the lattice plane and lattice row defining the cell of the twin lattice
O and M are successive lattice nodes along [uvw]
N = number of lattice planes of the family (hkl) from O to M
$X = |hu+kv+lw|$
n = twin index
$\mathbf{L}_{ind}$ is the lattice of the individual
$\mathbf{L}_{T}$ is the twin lattice

P-type lattice, twin plane (210), ⊥[210]



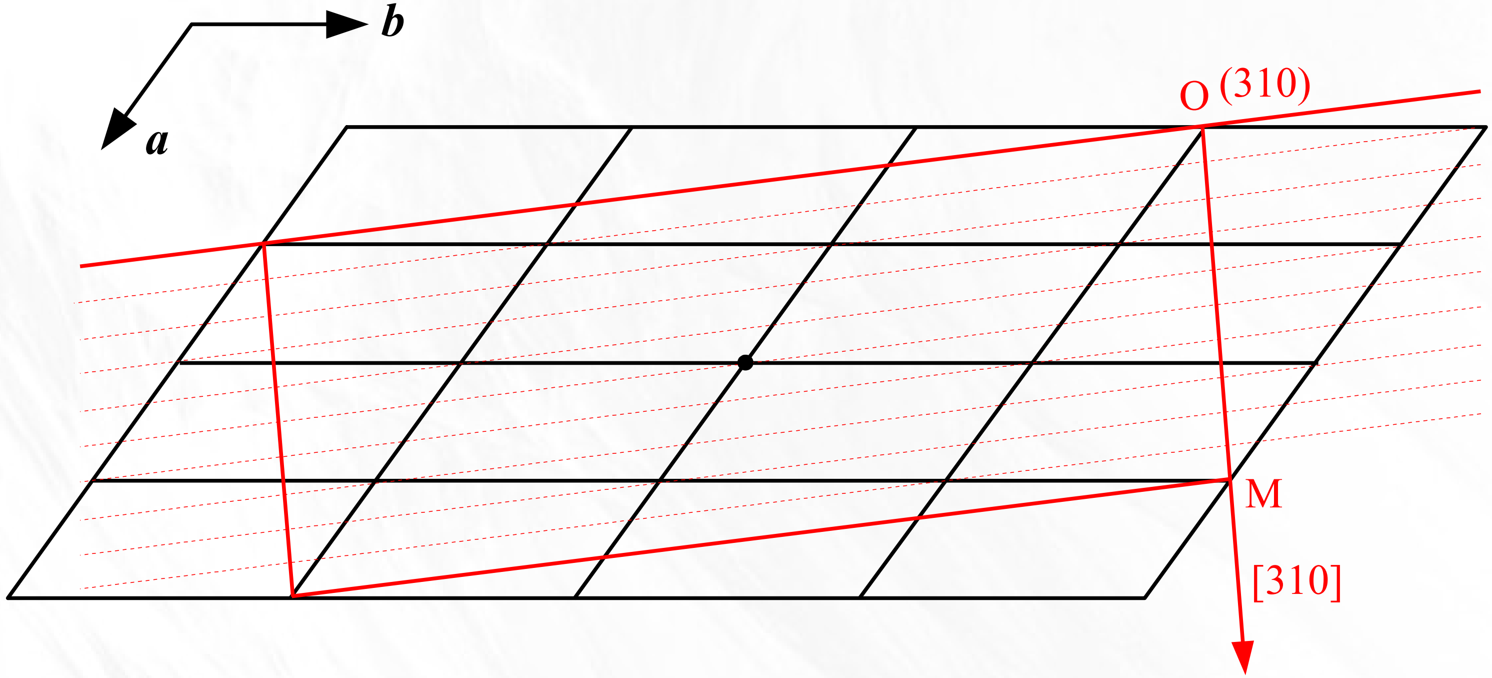
Only nodes at the corners of the red cell are restored.

There are $N = 5$ planes of the family (210) from O to M.

$X = 2\cdot2+1\cdot1+0\cdot0=5$

The twin index is $n = 5$ ($n = N = X$)

P-type lattice, twin plane (310), ⊥[310]

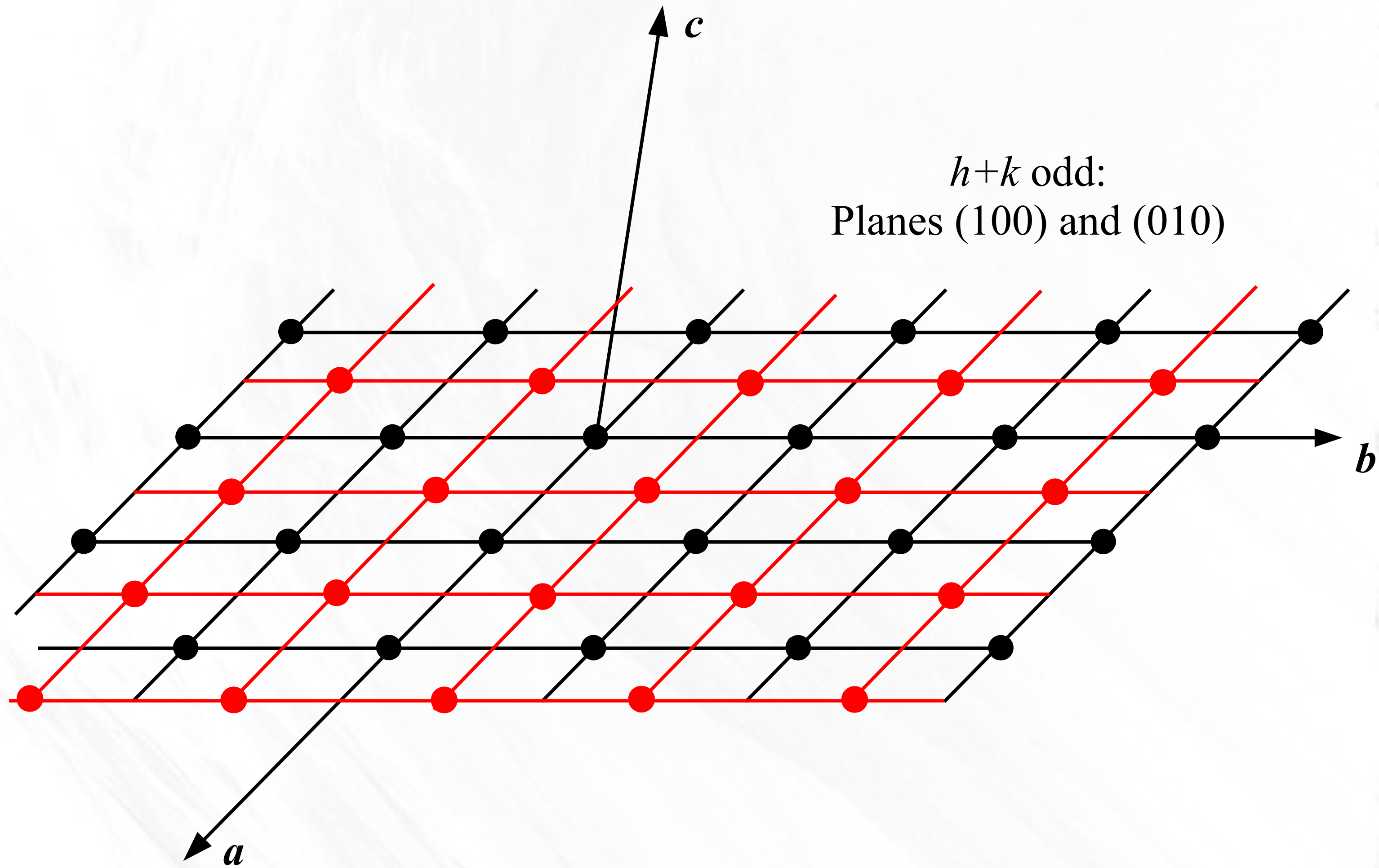


The nodes at the corners of the red cell and the node at the center are restored

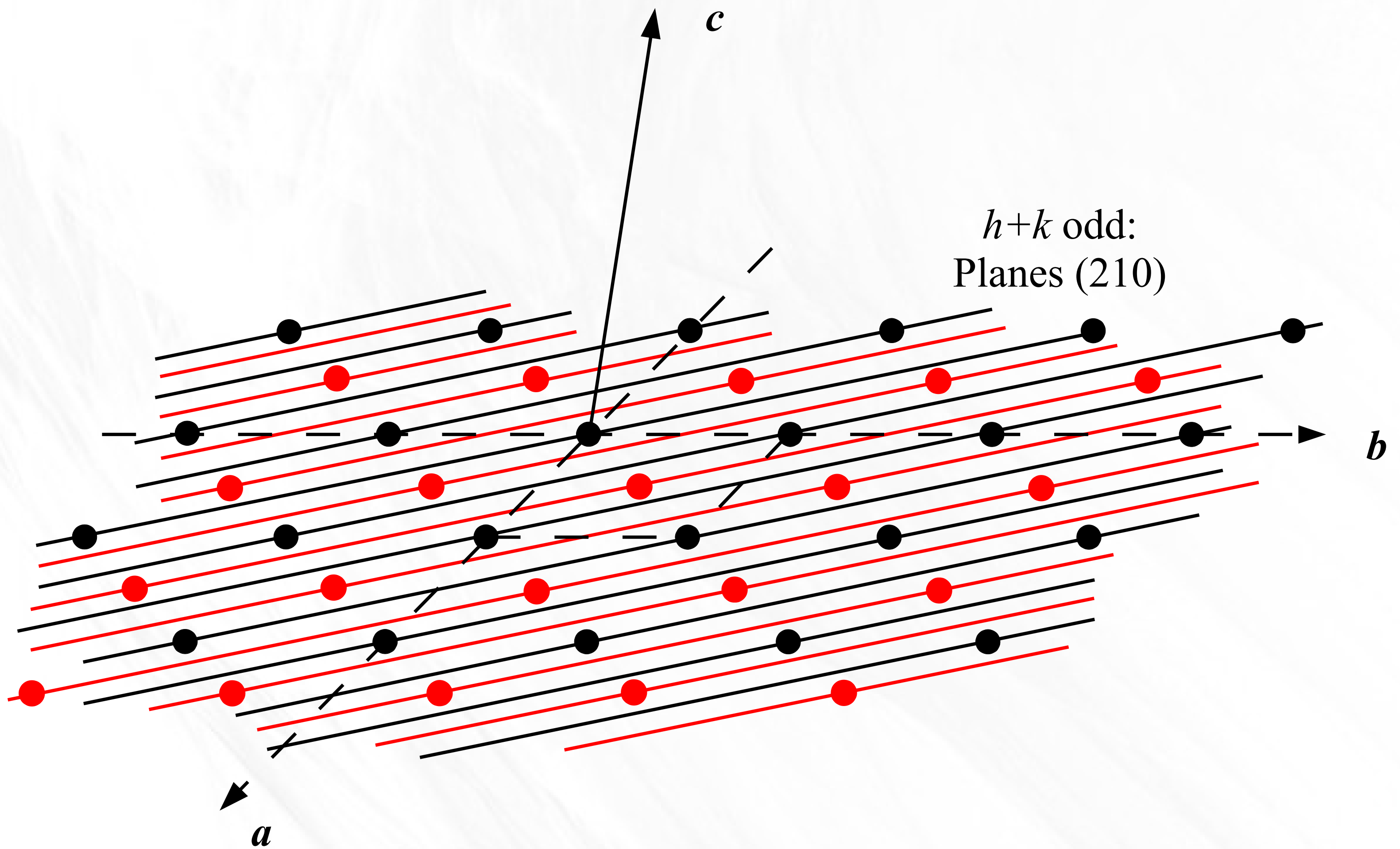
There are $N = 10$ planes of the family (310) between O and M.

$X = 3\cdot3+1\cdot1+0\cdot0=10$

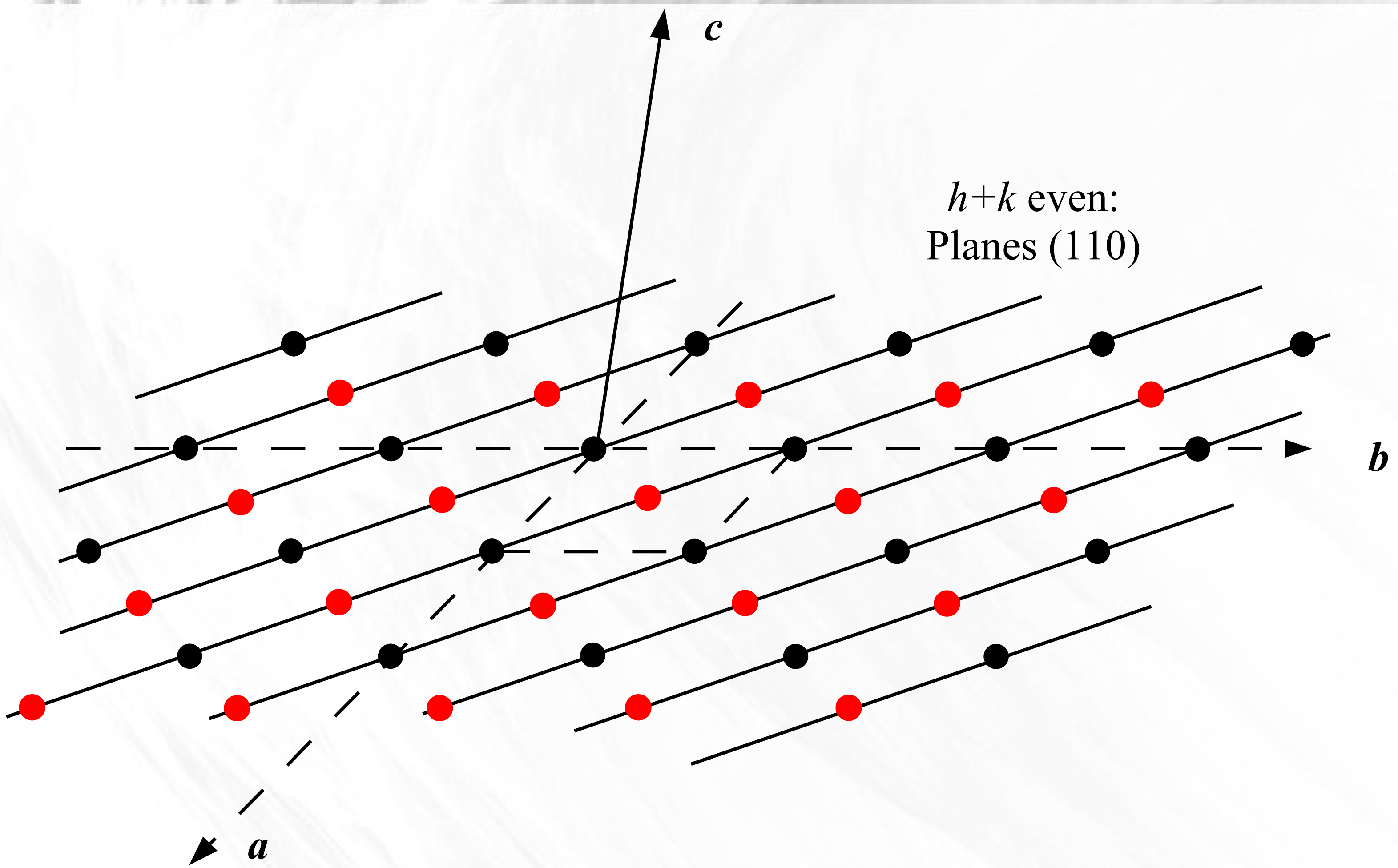
The twin index is $n = 5$ ($n = N/2 = X/2$)



Switching from *P* to *C* cell has no effect on the density of nodes on each plane but halves the interplanar distance



Switching from *P* to *C* cell has no effect on the density of nodes on each plane but halves the interplanar distance



Switching from *P* to *C* cell doubles the density of nodes on each plane but has no effect on the interplanar distance

We discover that...

(hkl) and [uvw] are the lattice plane and lattice row defining the cell of the twin lattice

O and M are successive lattice nodes along [uvw]

N = number of lattice planes of the family (hkl) from O to M

$X = |hu+kv+lw|$

n = twin index

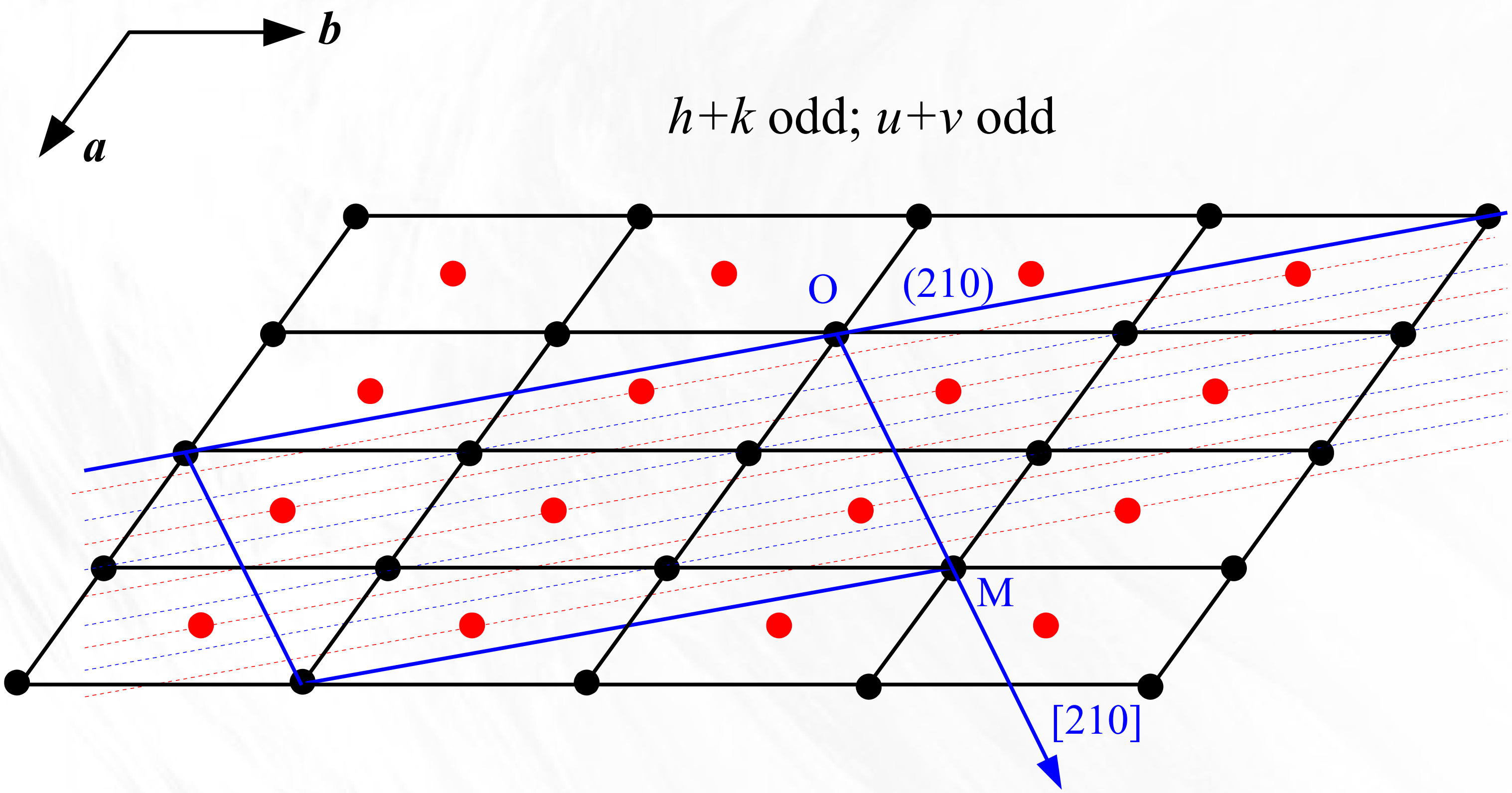
$\mathbf{L}_{ind}$ is the lattice of the individual

$\mathbf{L}_{T}$ is the twin lattice

For twofold twins, the two-dimensional coincidence index is either 1 or 0

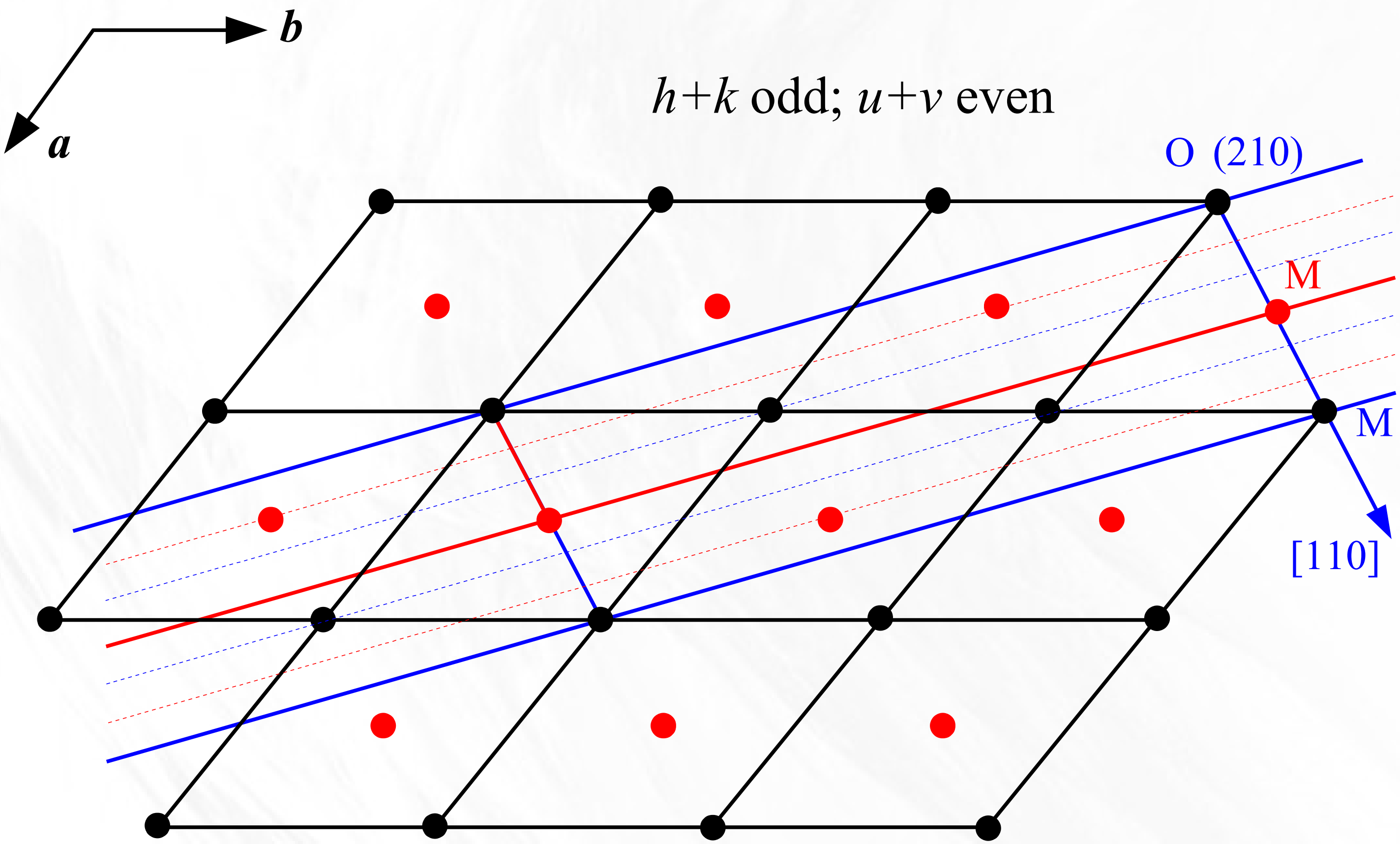
Let f be the number of lattice planes of the (hkl) family between O and M whose two dimensional coincidence index is 1

The twin index of twofold twins is simply $n = N/f$



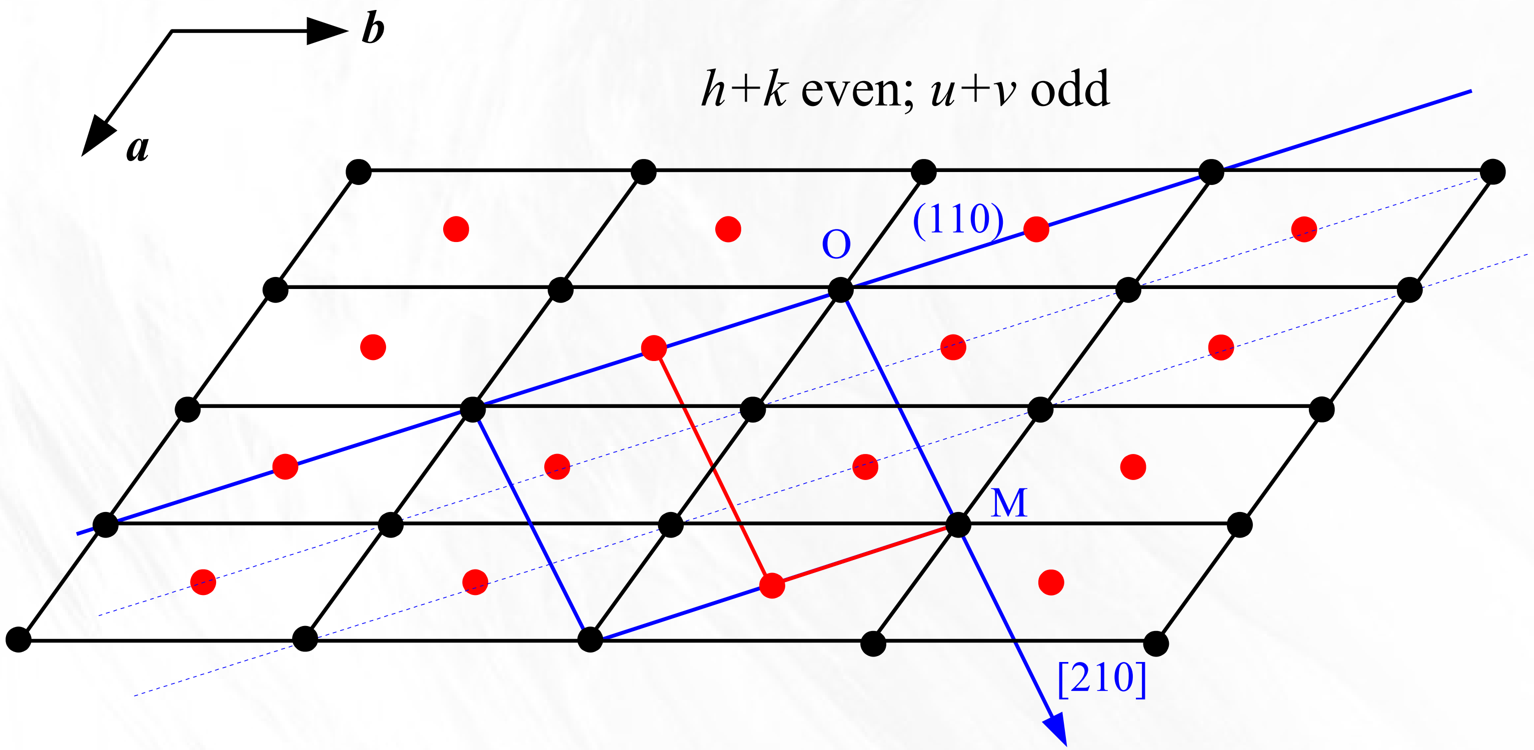
P type $\mathbf{L}_{\mathrm{ind}}$: $N = n = X = 5$, the cell of $\mathbf{L}_{\mathrm{T}}$ is primitive

C type $\mathbf{L}_{\mathrm{ind}}$: $N = 2X = 10$, $n = N/2 = X = 5$, the cell of $\mathbf{L}_{\mathrm{T}}$ is C-centered



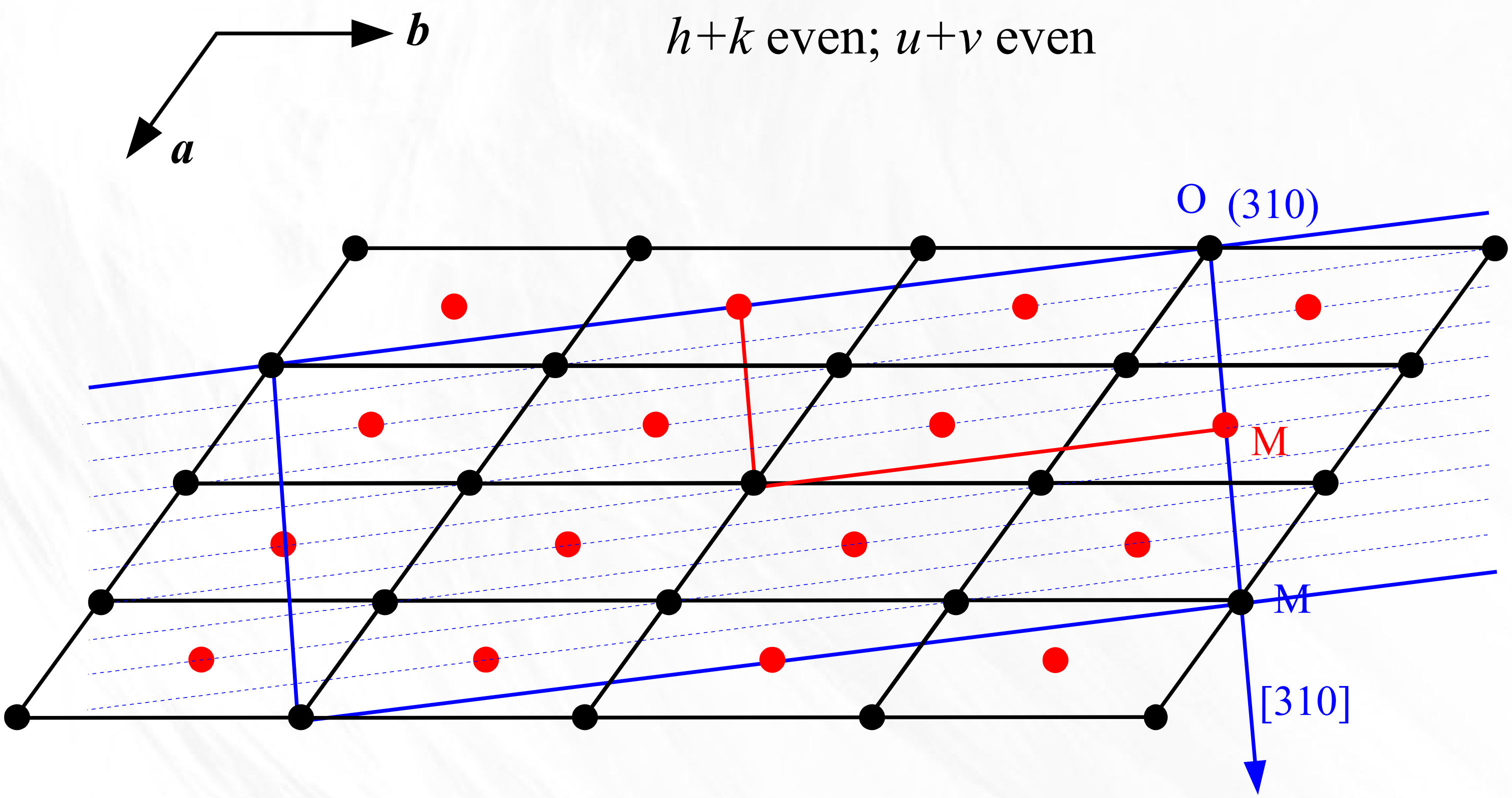
P type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive

C type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive and is twice smaller that that of *P* type $\mathbf{L}_{ind}$



P type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive

C type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive and is twice smaller that that of P type $\mathbf{L}_{ind}$



P type $\mathbf{L}_{ind}$: $N = X = 10$, $n = X/2 = 5$; the cell of $\mathbf{L}_T$ is *C*-centered

C type $\mathbf{L}_{ind}$: $N = n = X/2 = 5$, the cell of $\mathbf{L}_T$ is primitive and is twice smaller that that of *P* type $\mathbf{L}_{ind}$

Summarizing....

Computation of the twin index for twofold twins

- N = number of lattice planes of the family (hkl) between two successive lattice nodes along $[uvw]$
- n = twin index

Primitive cell

Conditions on *h,k,l*	**Conditions on *u,v,w***	***N***	***n***
none	none	X	if X is odd: $n = X$
			if X is even: $n = X/2$

C-centered cell

Conditions on *h,k,l*	**Conditions on *u,v,w***	***N***	***n***
$h+k$ odd	$u+v$ and w not both even	$2X$	$n = X$
	$u+v$ and w both even	X	$n = X$
$h+k$ even	$u+v$ and w not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$u+v$ and w both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

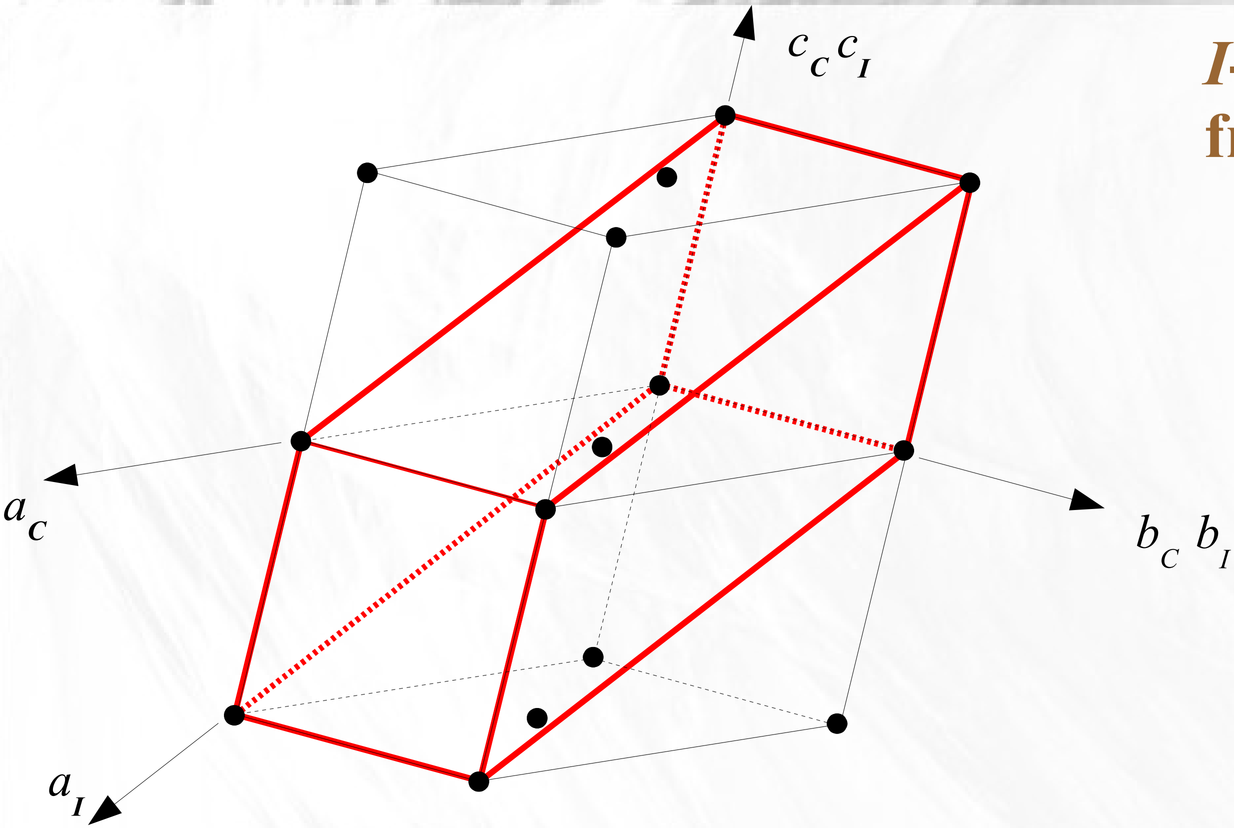
B-centered cell

Conditions on *h,k,l*	**Conditions on *u,v,w***	***N***	***n***
$h+l$ odd	$u+w$ and v not both even	$2X$	$n = X$
	u+w and v both even	X	$n = X$
$h+l$ even	u+w and v not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$u+w$ and v both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

A-centered cell

Conditions on *h,k,l*	**Conditions on *u,v,w***	***N***	***n***
$k+l$ odd	$v+w$ and u not both even	$2X$	$n = X$
	v+w and u both even	X	$n = X$
$k+l$ even	v+w and u not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$v+w$ and u both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

I-centered cell from a *C*-centered cell



Conditions on ***h,k,l***	Conditions on ***u,v,w***	***N***	***n***
$h+k+l$ odd	u, v, w not all odd	$2X$	$n = X$
	u, v, w all odd	X	$n = X$
$h+k+l$ even	u, v, w not all odd	X	X odd: $n = X$
			X even: $n = X/2$
	u, v, w all odd	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

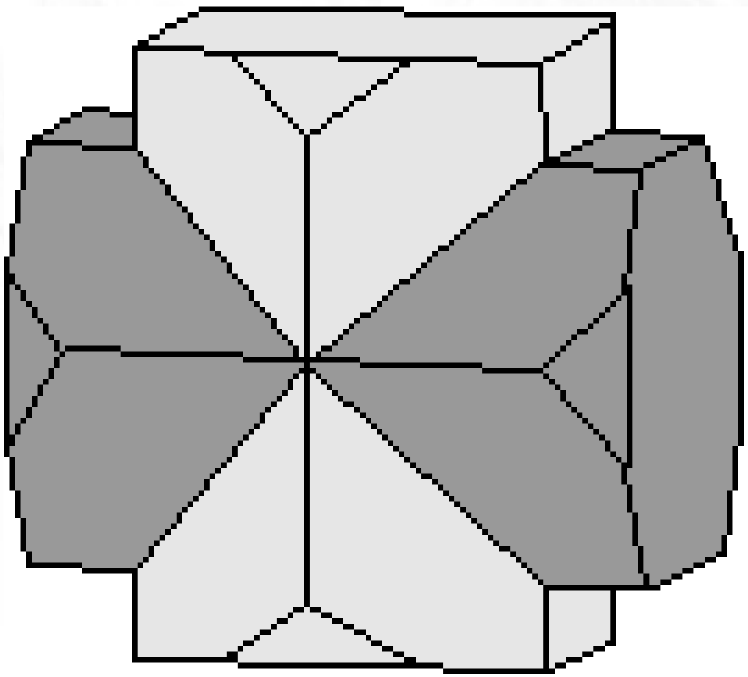
F-centered cell

F and *I* lattice types are one the dual of the other. The conditions for an *I*-centered cell apply also to an *F*-centered cell provided that (*hkl*) and [*uvw*] are exchanged.

Conditions on *h,k,l*	**Conditions on *u,v,w***	***N***	***n***
h, k, l not all odd	$u+v+w$ odd	$2X$	$n = X$
h, k, l all odd	u, v, w all odd	X	$n = X$
h, k, l not all odd	$u+v+w$ even	X	X odd: $n = X$
			X even: $n = X/2$
h, k, l all odd		$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

What about manifold twins?

Greek-cross fourfold-twin in staurolite



$C2/m$

$a = 7.871$ Å

$b = 16.620$ Å

$c = 5.656$ Å

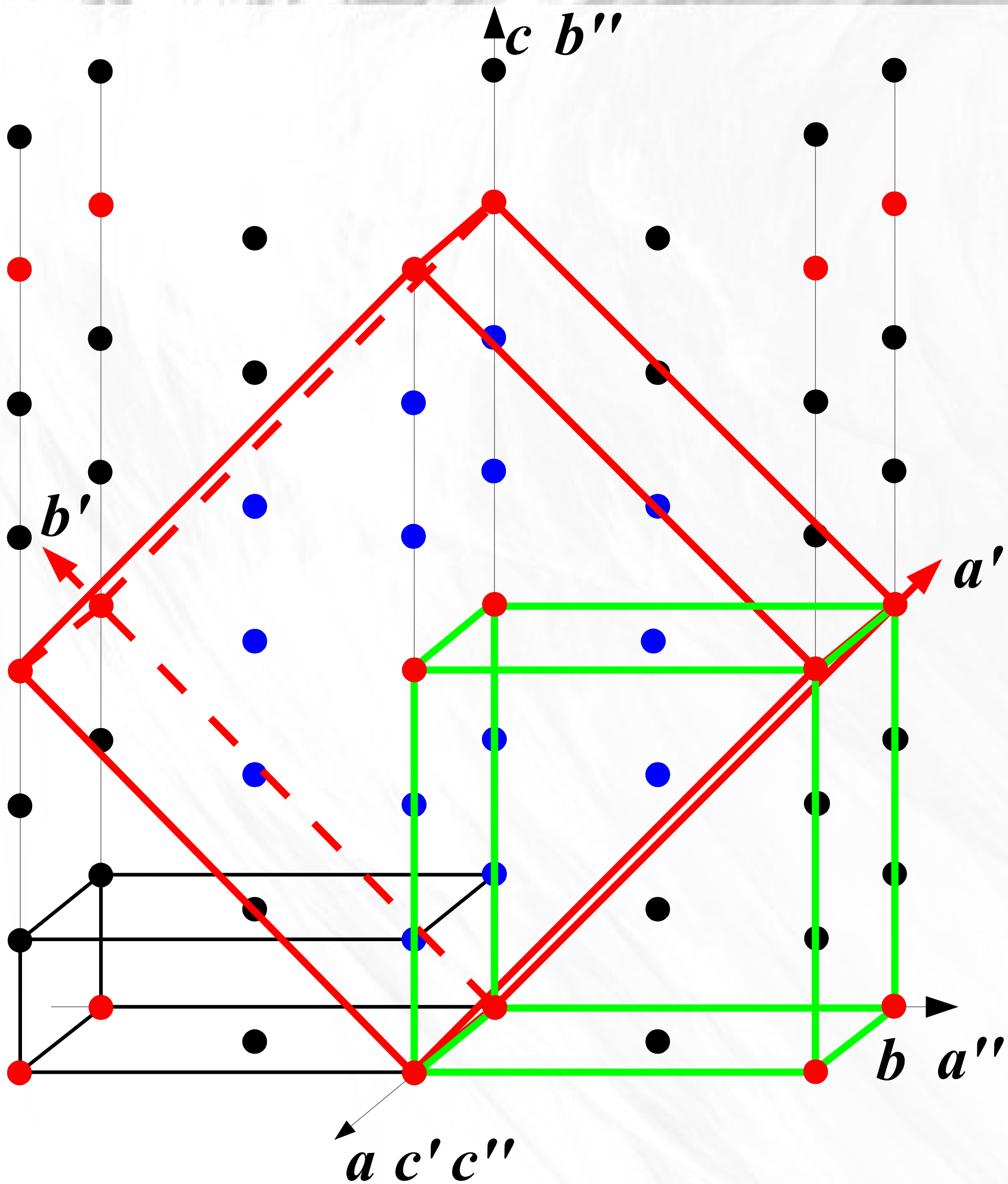
$\beta = 90^{\circ}$

Twin operation: $4_{[100]}$

[100] is perpendicular to (100)

$$X = |1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0|$$

Is the twin index 1?



12 nodes in the *tC* cell of $\mathbf{L}_T$: the twin index is 6

tC is not a standard cell – let us transform it to the standard *tP* cell

6 nodes in the *tP* cell of $\mathbf{L}_T$: the twin index is 6

no nodes at all restored on this plane

2 nodes out of 6 restored on this plane (restoration index is 3)

1 plane of the (100) family out of 2 has a coincidence index of 3

$n = 2 \cdot 3 / 1 = 6$

How to compute the twin index of a manifold twin?

- Let N be the number of lattice planes of the (hkl) family passing within the cell of the twin lattice.
- Out of these N planes, ξ be the number of planes that are partially restored by the twin operation (the other N-ξ are not restored at all).
- Let Ξ be the reciprocal of the two-dimensional coincidence index for a plane of the (hkl) family that is partially restored by the twin operation

The twin index is $n = N\Xi/\xi$

Cumbersome? Than take a shorter route:

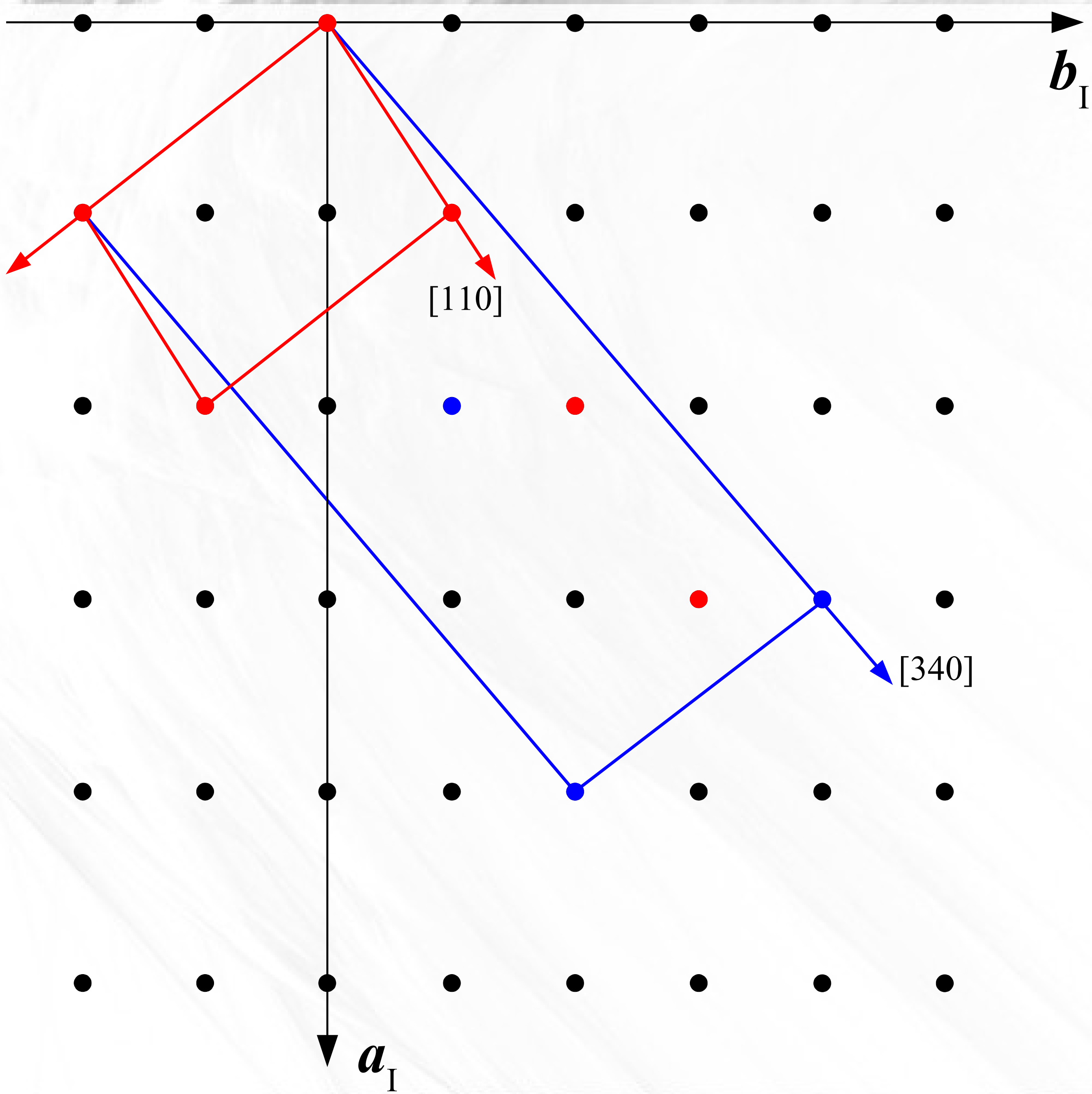
Find a twofold operation in the same coset and apply the classical formula!

Beyond the classical reticular theory of twins

Hybrid twins:
somebody chooses one out of N - we take them all!

Friedelian twins

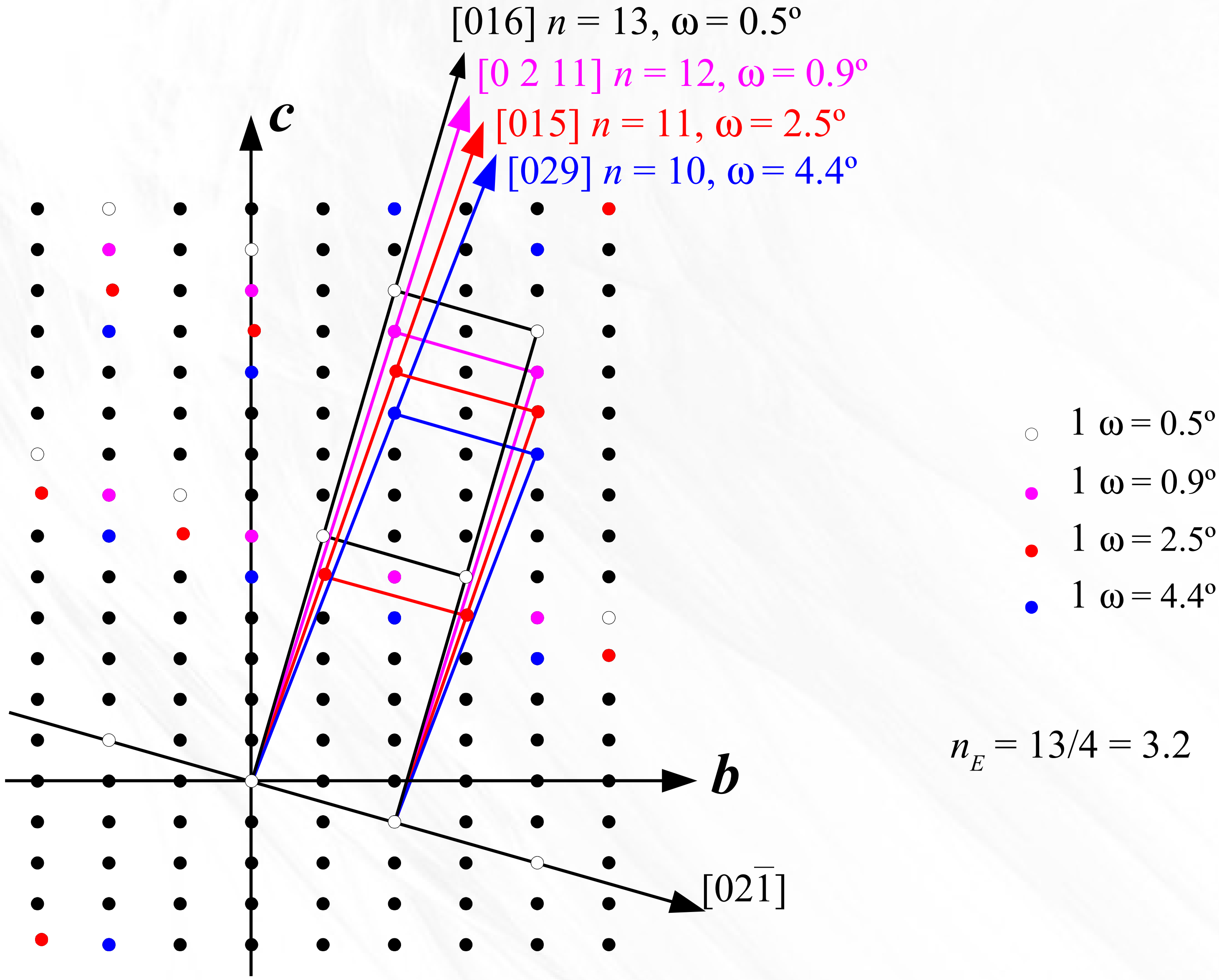
- The probability of occurrence on a twin is inversely proportional to the twin index and to the obliquity
- Friedel's empirical criterion: $n \leq 6$, $\omega \leq 6^{o}$
- Twins for which the above criterion is obeyed are termed “Friedelian twins”



uvw	ω	*n*
110	5.36º	3
~~230~~	~~5.86º~~	~~7~~
340	2.50º	5
~~450~~	~~0.69º~~	~~13~~

Effective twin index: 10/(4+1) = 2.0

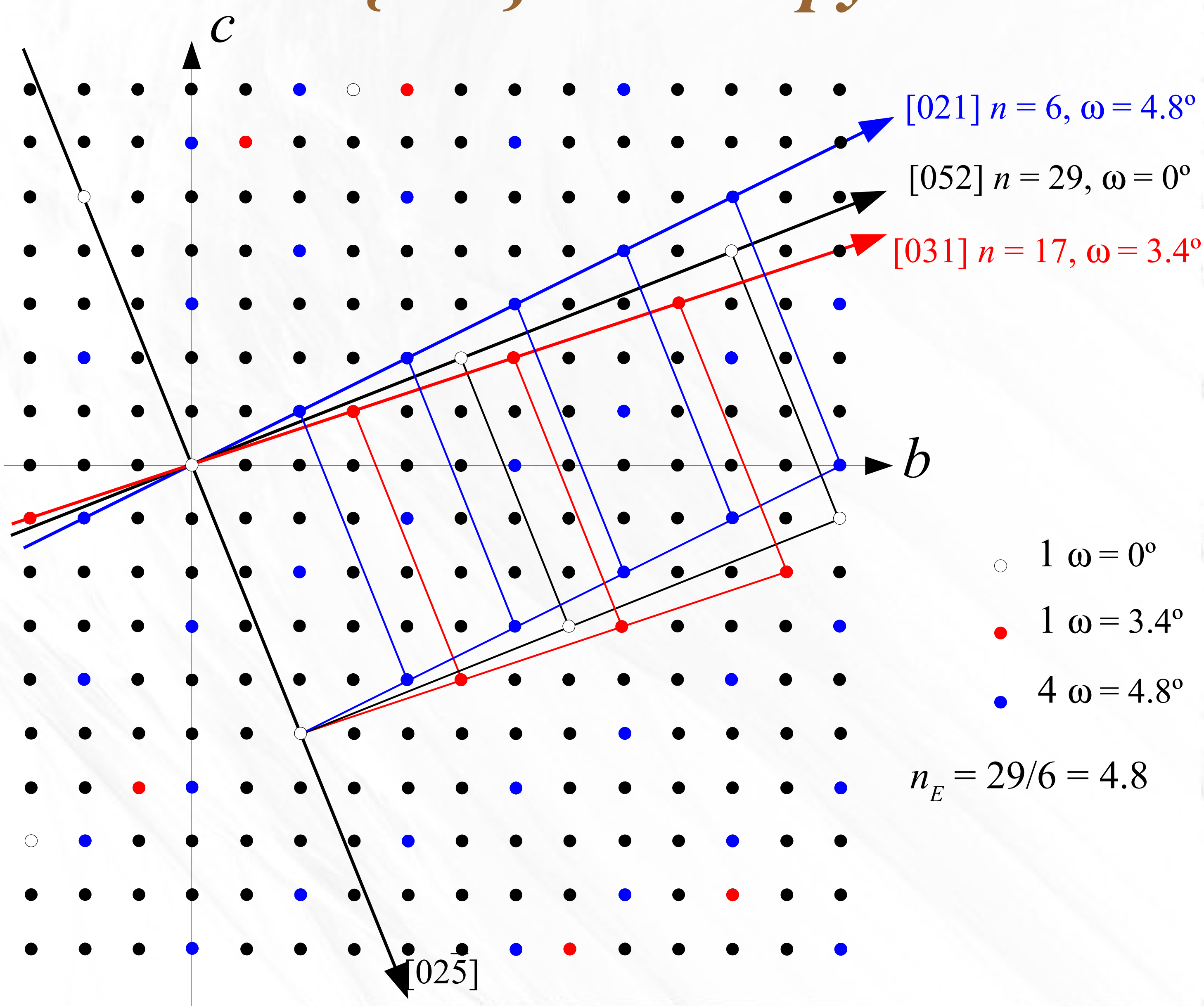
{012} twin in forsterite Pbnm



$n_E = 13/4 = 3.2$

{052} twin in pyrite $Pa\bar{3}$

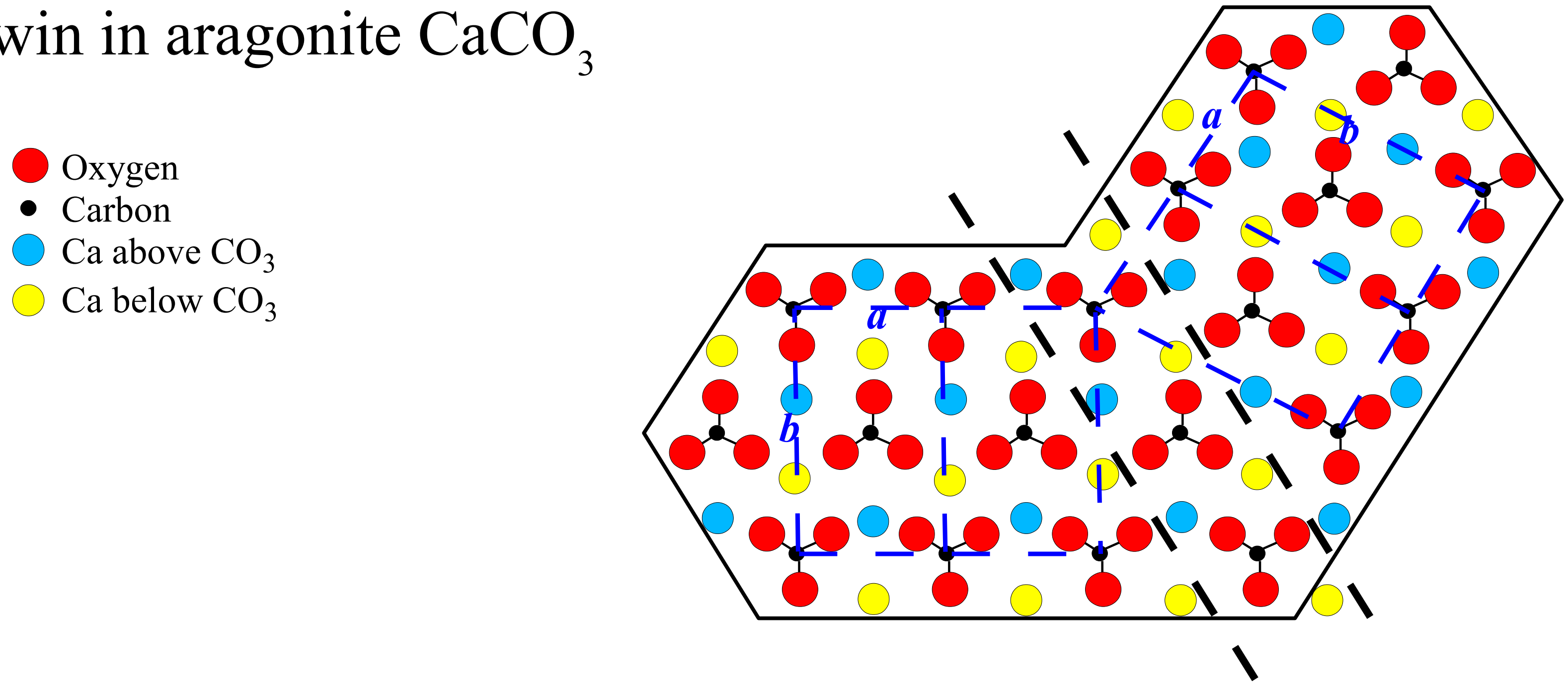
In a cubic lattice, for each (*hkl*) plane there is a direction [*hkl*] exactly perpendicular



$n_E = 29/6 = 4.8$

Towards a structural theory of twins

(110) twin in aragonite $CaCO_3$



Some of the atoms cross the interface without changing position: they produce a substructure common to the two orientations

A crystallographic orbit with eigensymmetry E higher than the space group G (extraordinary orbit) may possess among its symmetry operations one that maps the two orientations.

The slab shown in the figure is common to both orientations.

The diperiodic group obtained as sectional group of G in the orientation of the slab may have a higher symmetry than the intersection group of the space groups of the two individuals and include an operation that maps the two orientations.

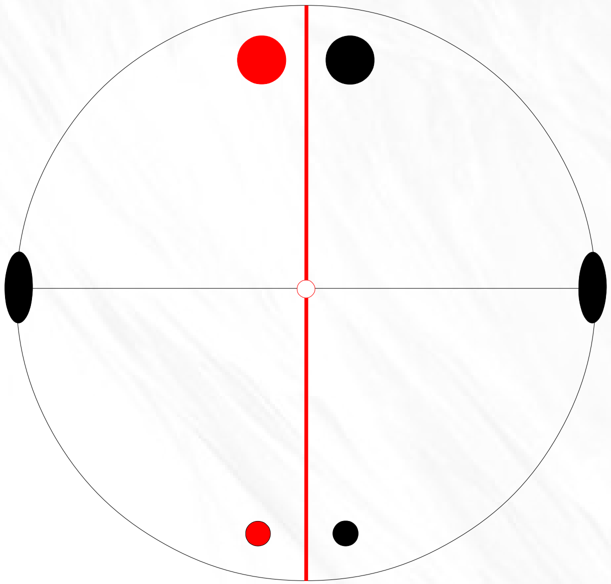
Twin point groups

Definitions

- Dichromatic crystallographic point groups: Shubnikov groups $K^{(2)}$
- Polychromatic invariant extension of crystallographic point groups: Koptsik groups $K^{(p>2)}$
- Polychromatic non-invariant extension of crystallographic point groups: Van der Waerden-Burckhardt groups $K_{WB}^{(p>2)}$

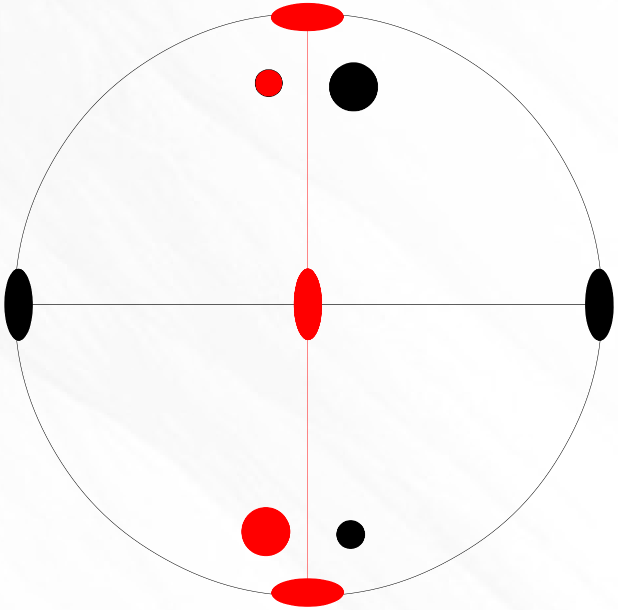
Example of dichromatic (Shubnikov) $K^{(2)}$ groups

H* = 2



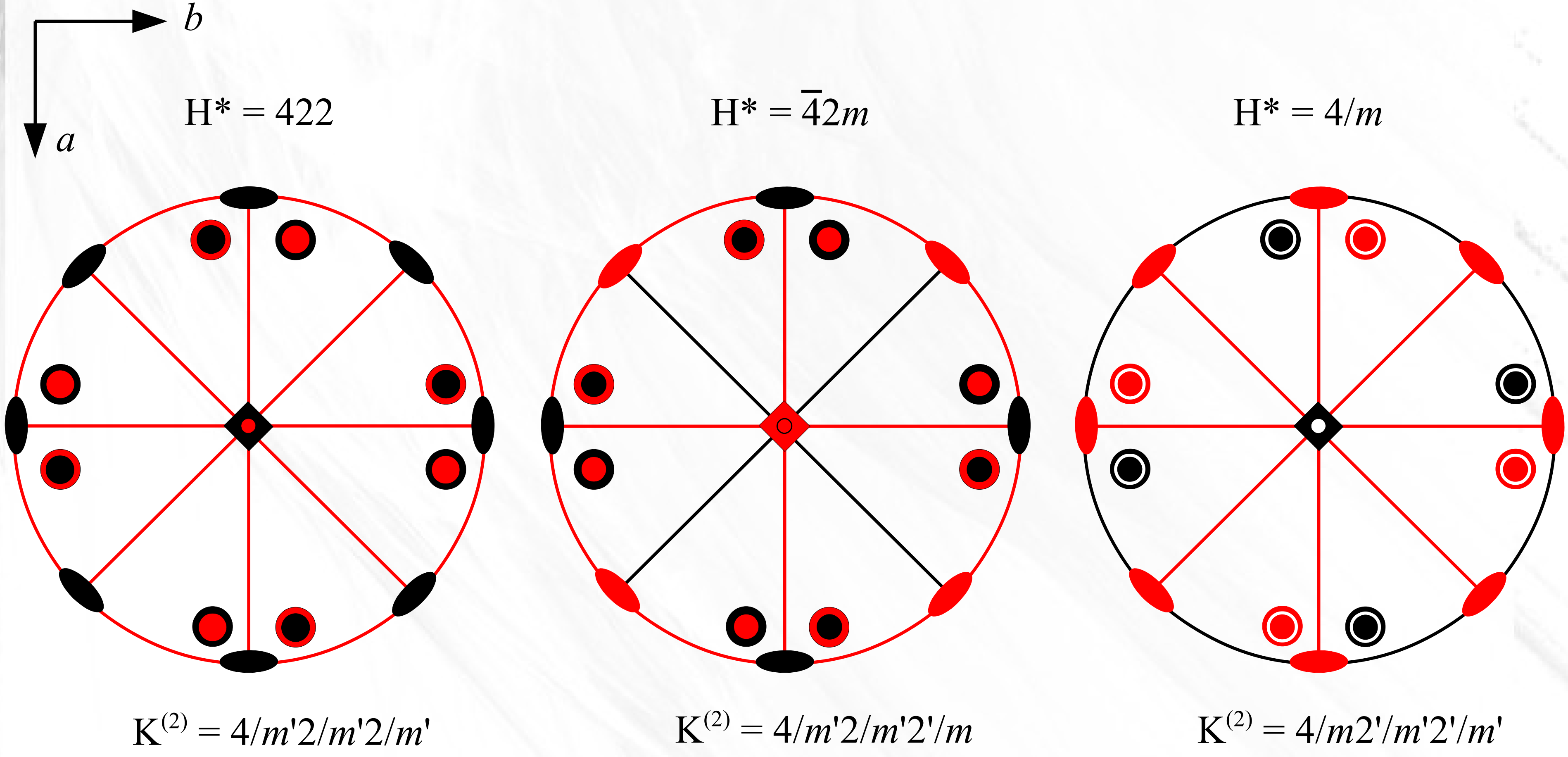
$K^{(2)} = 2/m'$

H* = 2

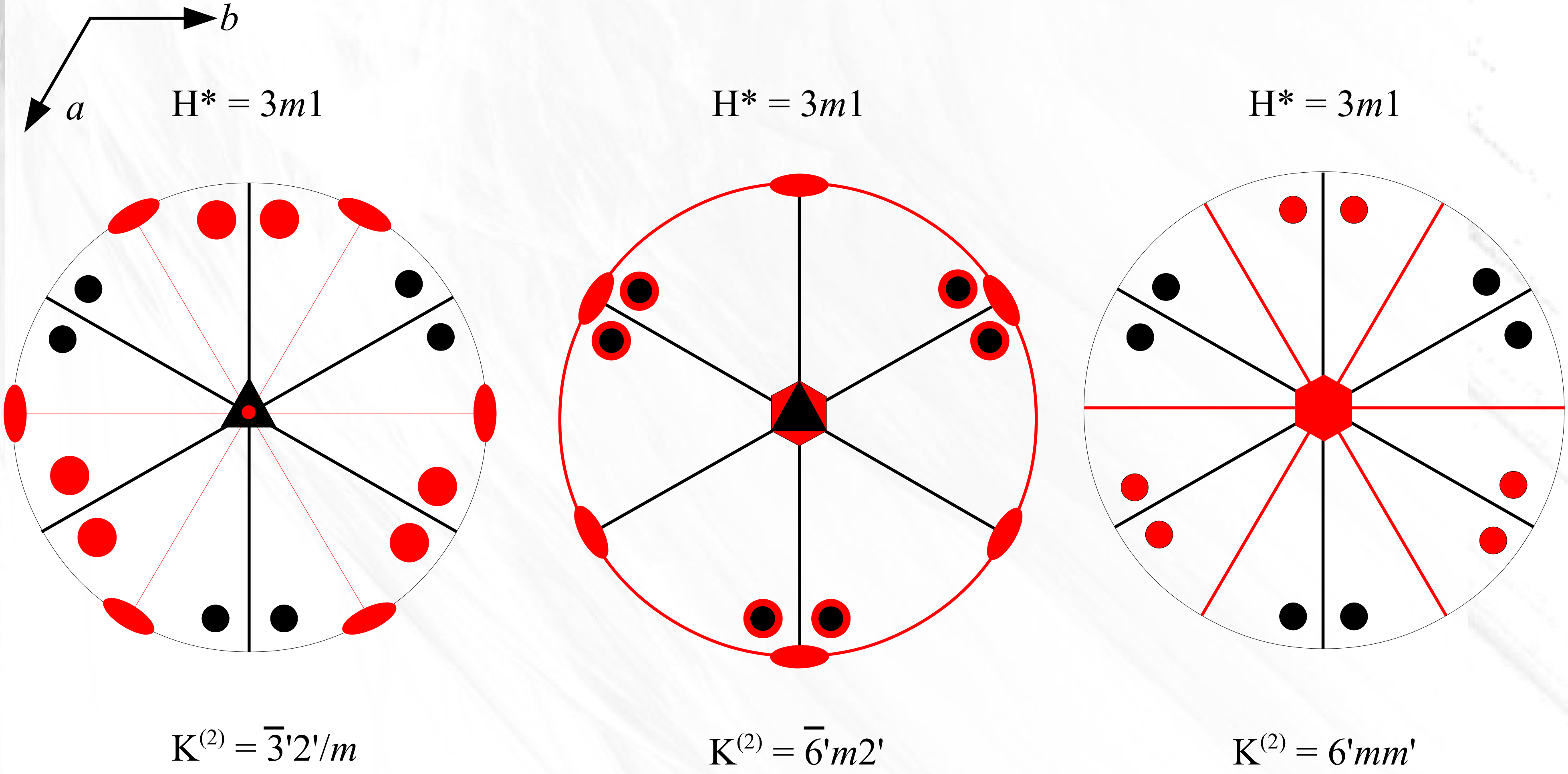


$K^{(2)} = 2'22'$

A simple exercise on dichromatic (Shubnikov) groups: three $K^{(2)}$ groups corresponding to the same holohedral achromatic group



A simple exercise on dichromatic (Shubnikov) groups: obtain the possible $K^{(2)}$ from the given H*



Exercise

Find the twin point group of two individuals with H = 222 related by a twin mirror plane (010). What type of twin is it?

Exercise

Find the twin point group of two individuals with H = 222 related by a fourfold twin axis parallel to [001]. What type of twin is it?

Exercise

Find the twin point group of two individuals with H = *mmm* related by a fourfold twin axis parallel to [001]. What type of twin is it?

Exercise

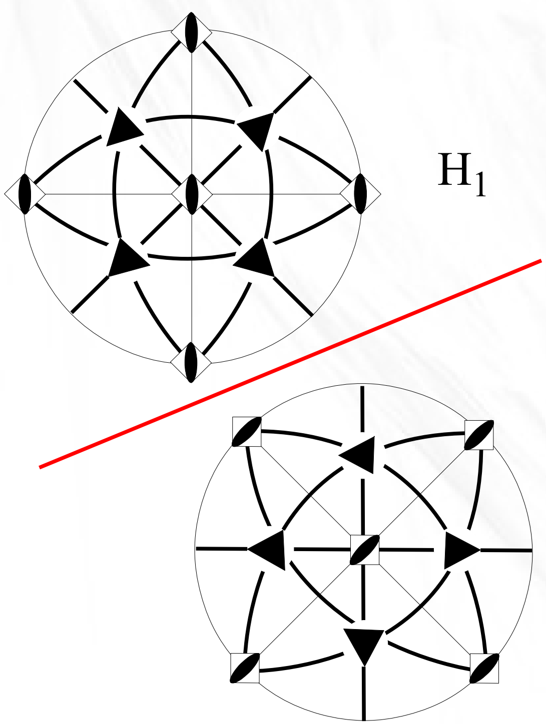
Find the twin point group of two individuals with H = 2 and $\beta = 90^{o}$ related by a twofold twin axis parallel to [100]. What type of twin is it?

Exercise

Find the twin point group of two individuals with H = m and $\beta = 90^{\circ}$ related by a twofold twin axis parallel to [100]. What type of twin is it?

Exercise

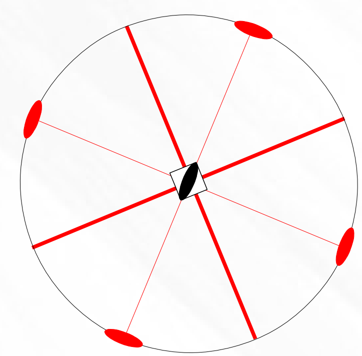
(210) twinning in hauyne, $H = \bar{4}3m$



H_1

H_2

$H^* = \bar{4}$



$K = \bar{4}2'm'$

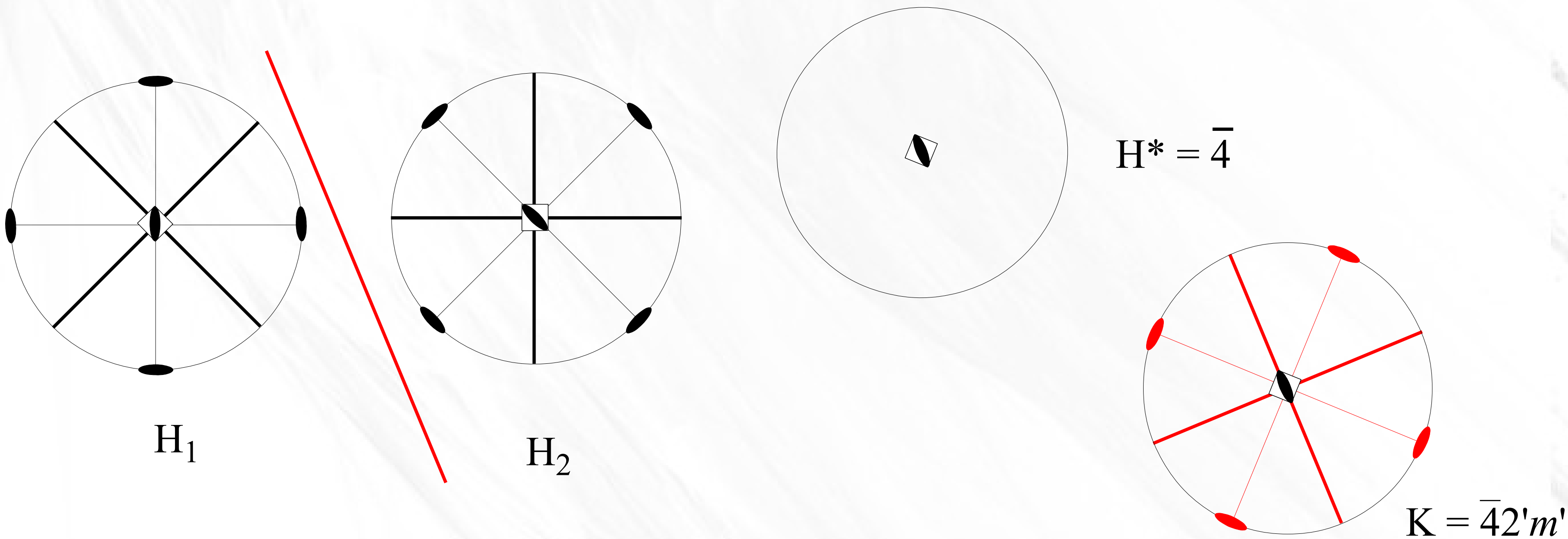
Twinning by reticular merohedry

What is the twin index?

$K \subset H$

Exercise

$(\bar{1}20)$ twinning in melilite, H = $\bar{4}2m$

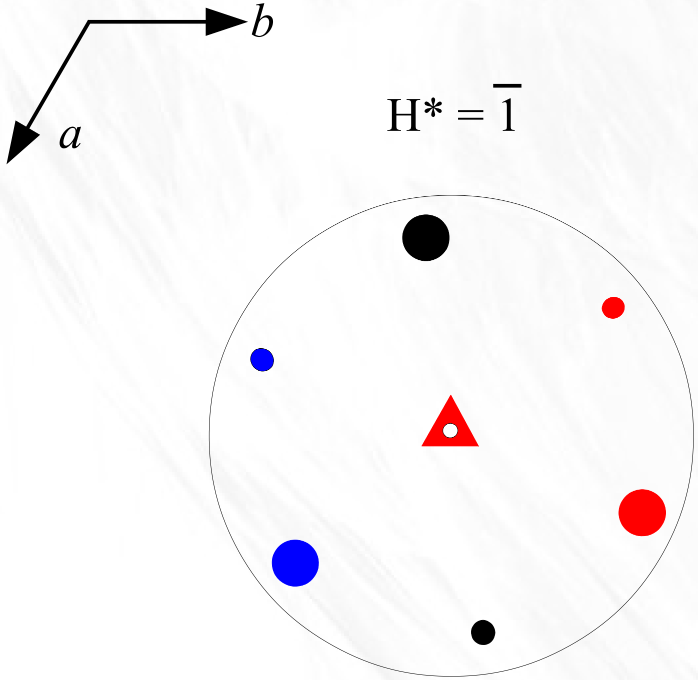


Twinning by reticular polyholohedry

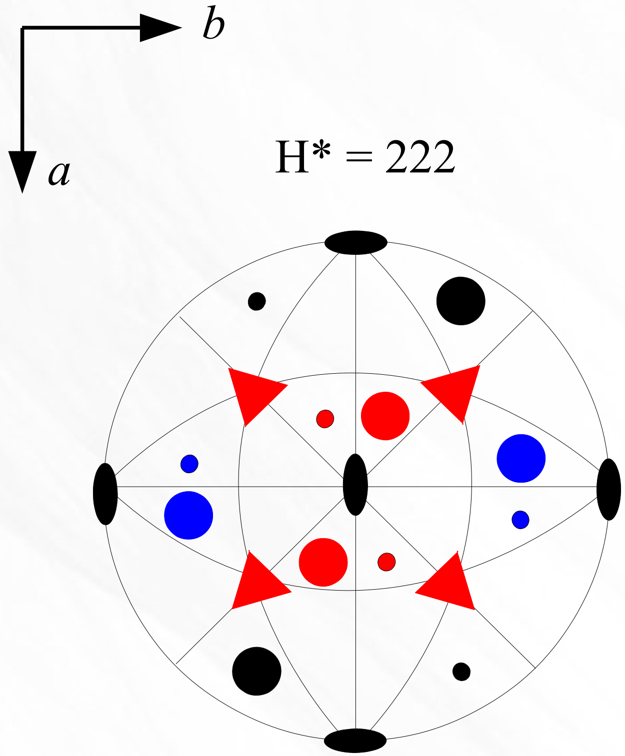
What is the twin index?

K = H

Examples of Koptsik $K^{(p)}$ groups for first-order twins

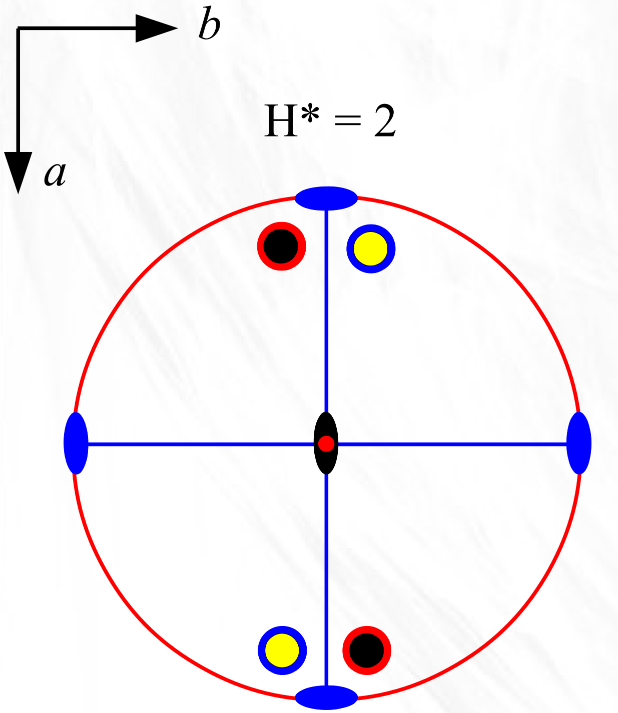


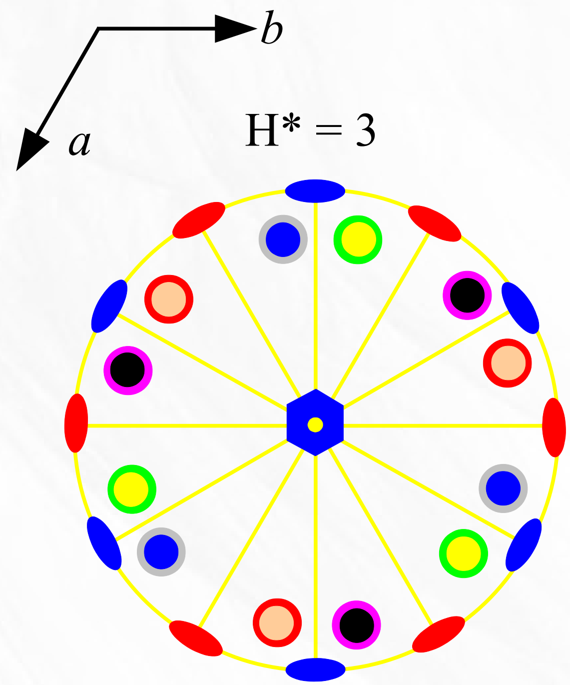
$K^{(3)} = \bar{3}^{(3)}$



$K^{(3)} = (23^{(3)})^{(3)}$

Examples of Koptsik $K^{(p)}$ groups for higher-order twins





$K^{(2)}=2/m'$

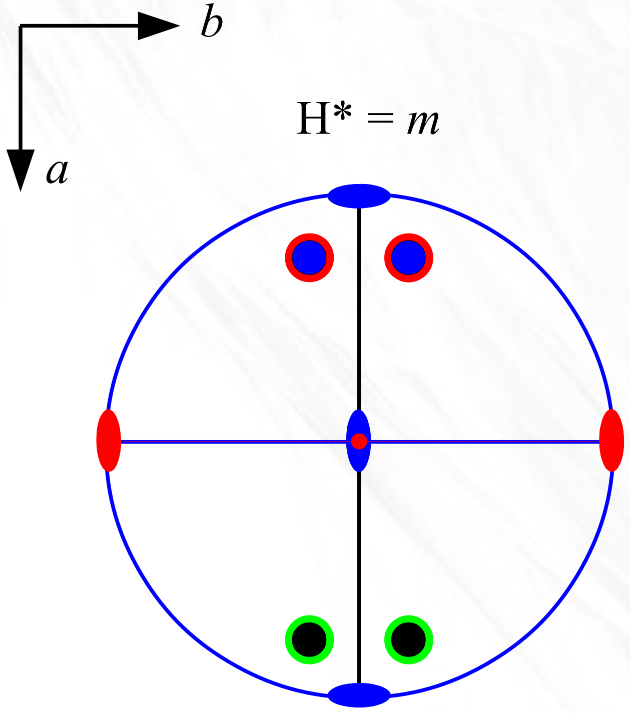
$$K^{(4)}=\left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2}{m^{(2)}}\right)^{(4)}$$

$K^{(2)}=32'1 \longrightarrow K^{(4)}=(6^{(2)}2^{(2)}2^{(2)})^{(4)}$

$$K^{(8)}=\left(\frac{6^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$$

A simple exercise on Koptsik groups: obtain the possible holohedral $K^{(p>2)}$ from $H^* = m$

I: orthorhombic $K^{(p)}$



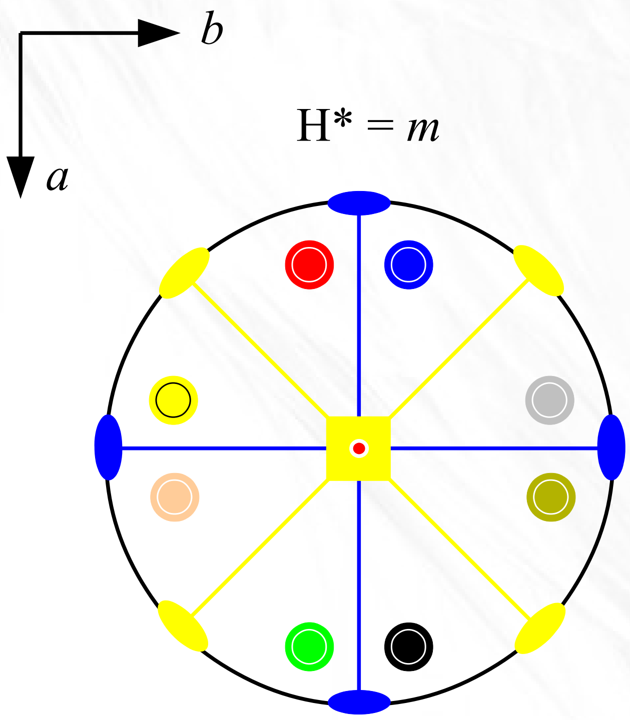
$K^{(2)}=2'/m$

↓

$$K^{(4)}=\left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$$

A simple exercise on Koptsik groups: obtain the possible holohedral $K^{(p>2)}$ from $H^* = m$

II: tetragonal $K^{(p)}$



$K^{(2)} = 2'/m$

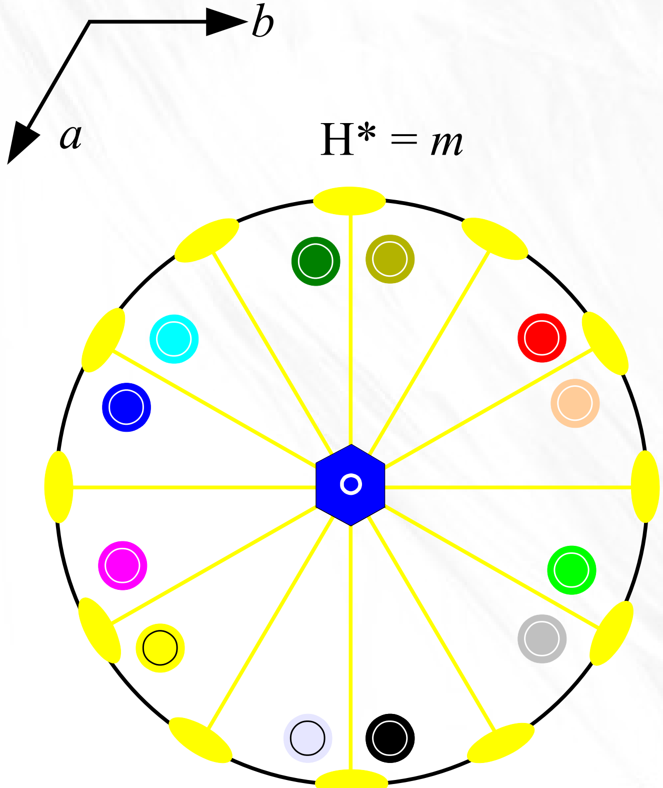
$$K^{(4)} = \left(\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m}\right)^{(4)}$$

$$K^{(8)} = \left(\frac{4^{(4)}}{m}\frac{2^{(2)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2)}}\right)^{(8)}$$

Note the change of axial setting!

A simple exercise on Koptsik groups: obtain the possible holohedral $K^{(p>2)}$ from $H^* = m$

III: hexagonal $K^{(p)}$



$$K^{(3)} = \bar{6}^{(3)}$$

$$\downarrow$$

$$K^{(6)} = \left(\frac{6^{(6)}}{m}\right)^{(6)}$$

$$\downarrow$$

$$K^{(12)} = \left(\frac{6^{(6)}}{m}\,\frac{2^{(2)}}{m^{(2)}}\,\frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$$

Exercise

Find the twin point group of four individuals with H = 2 related by 1) a mirror plane (010) and 2) a twofold twin axis parallel to [100]. What type of twin is it?

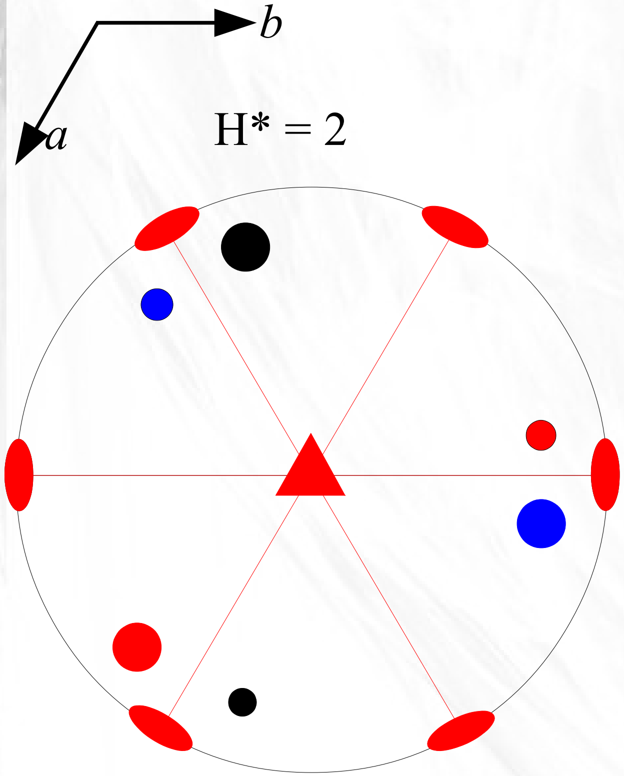
Exercise

Find the twin point group of three individuals with H = 2 related by a threefold twin axis parallel to [010]. What type of twin is it? What happens if one of the individuals does not develop or is chopped off?

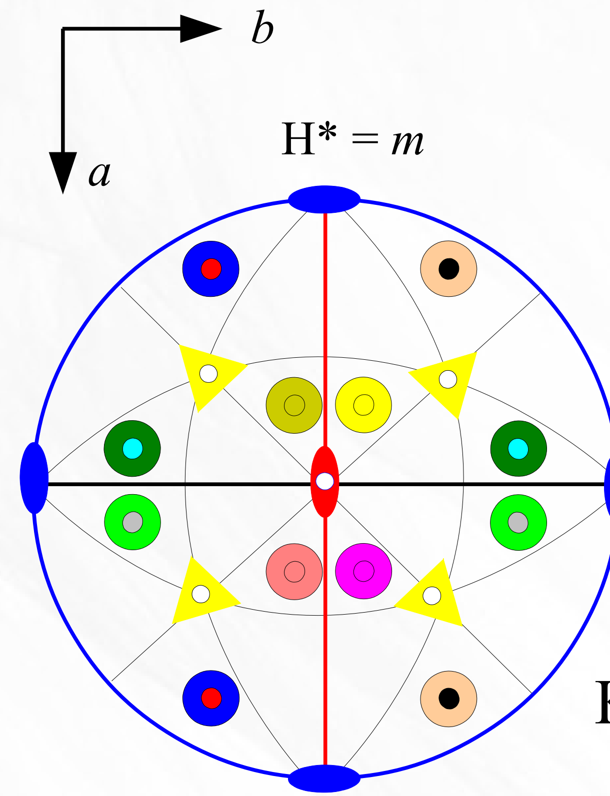
Exercise

Repeat the previous exercise by adding:
➔a twin mirror plane (001)
➔a twofold twin axis parallel to [100]
What type of twin is it? What happens if two of the individuals do not develop or are chopped off?

Examples of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups



$$K_{WB}^{(3)} = (3^{(3)}2^{(2,1)})^{(3)}$$

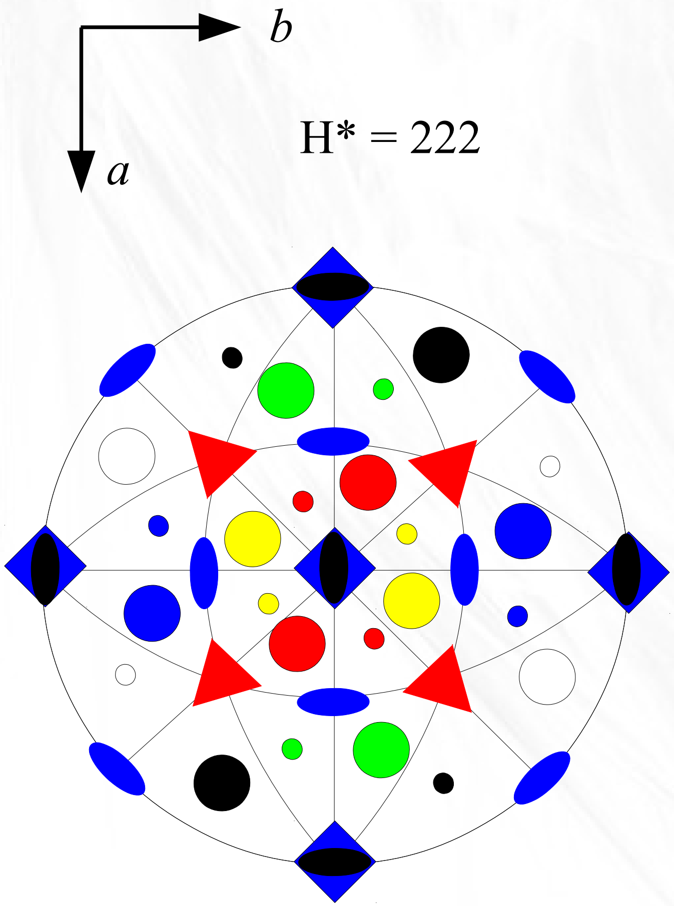


$$K^{(2)} = m'm2'$$

$$K^{(4)} = \left(\frac{2^{(2)}}{m} \frac{2^{(2)}}{m^{(2)}} \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}$$

$$K_{WB}^{(12)} = \left(\frac{2^{(2)}}{m^{(2,4)}} \bar{3}^{(6)} \right)^{(12)}$$

Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups with partially chromatic element over a chromatic element

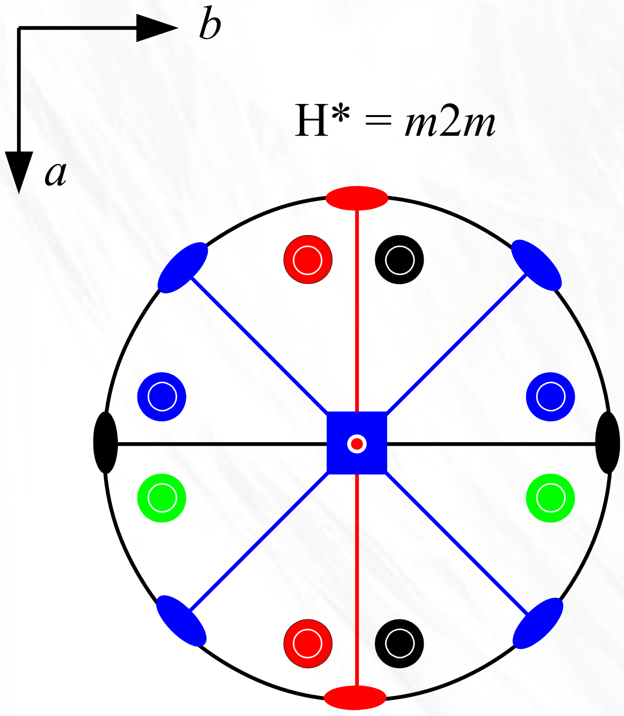


$$K^{(3)}=(23^{(3)})^{(3)}$$

$$\downarrow$$

$$K_{WB}^{(6)}=(4^{(4,0)}3^{(3)}2^{(2,2)})^{(6)}$$

Example of Van der Waerden-Burckhardt $K_{WB}^{(p)}$ groups for higher-order twins



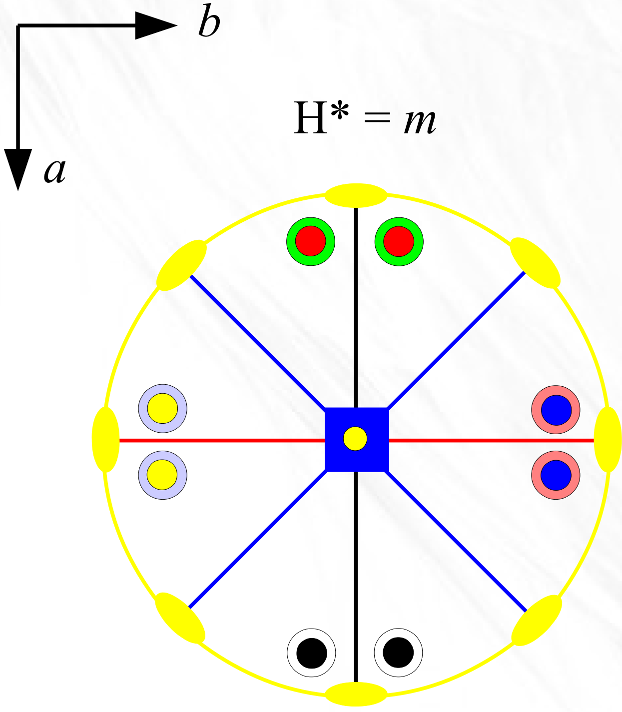
$$K' = \left(\frac{2'}{m} \; \frac{2}{m'} \; \frac{2'}{m} \right)$$

$$\downarrow$$

$$K_{WB}^{(4)} = \left(\frac{4^{(4)}}{m} \; \frac{2^{(2,2)}}{m^{(2,2)}} \; \frac{2^{(2)}}{m^{(2)}} \right)^{(4)}$$

A simple exercise on Van der Waerden-Burckhardt groups: obtain the possible holohedral $K_{WB}^{(p>2)}$ from $H^* = m$

I: tetragonal $K_{WB}^{(p)}$



$K^{(2)}=m'm2'$

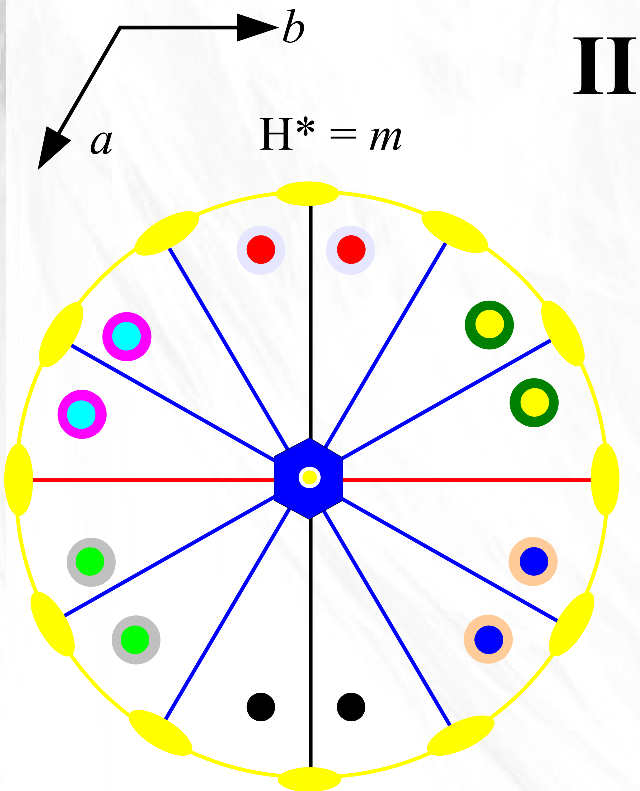
↓

$K_{WB}^{(4)}=(4^{(4)}\ m^{(2,2)}m^{(2)})^{(4)}$

↓

$$K_{WB}^{(8)}=\left(\frac{4^{(4)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2,4)}}\ \frac{2^{(2)}}{m^{(2)}}\right)^{(4)}$$

A simple exercise on Van der Waerden-Burckhardt groups: obtain the possible holohedral $K_{WB}^{(p>2)}$ from $H^* = m$



II: hexagonal $K_{WB}^{(p)}$

$K^{(2)}=m'm2'$

↓

$K_{WB}^{(6)}=(6^{(6)}m^{(2,2)}m^{(2)})^{(6)}$

↓

$$K_{WB}^{(12)}=\left(\frac{6^{(6)}}{m^{(2)}}\frac{2^{(2)}}{m^{(2,4)}}\ \frac{2^{(2)}}{m^{(2)}}\right)^{(12)}$$