Workshop on crystal twinning

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What is a twin?

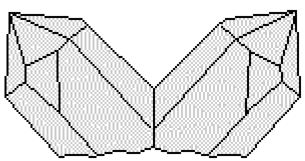
With space group

No space group

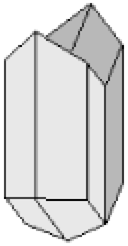
A twin is a heterogeneous edifice built by homogeneous crystals (individuals) of the same phase in different orientations, related by an operation (the twin operation) that does not belong to the point group of the individual.

Georges Friedel, 1904

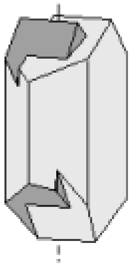
Mapping of individuals in twins



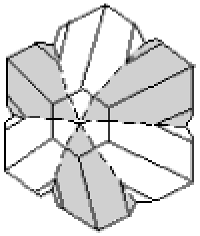
Reflection in {11$\bar{2}$2}



Reflection in (100)



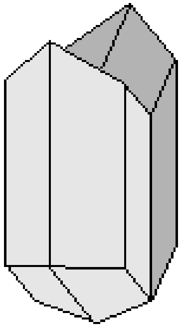
Rotation about [001]



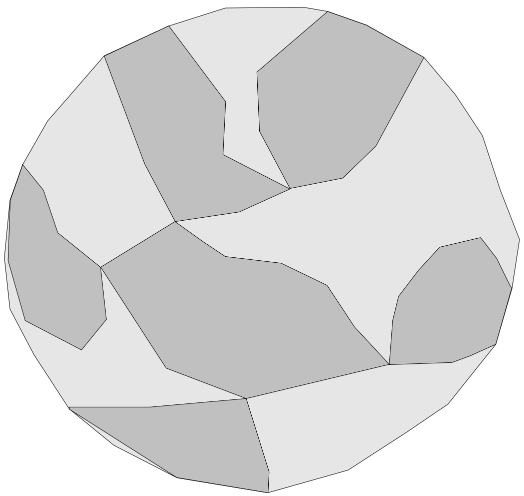
Reflection in {031} (cyclic twin)

Twinning is a point-group phenomenon

Basic definitions



Two individuals

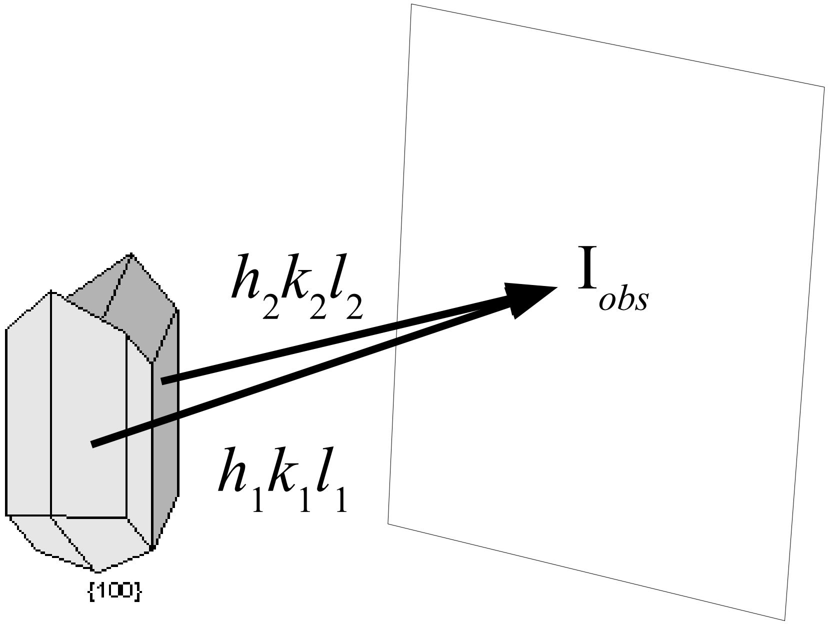


Two orientation domains (domain states, variants) with N domains

Problems related to twins. I. Effects of twinning on the diffraction pattern.

- Because twinning is a point group phenomenon, intensities from twins do not interfere but simply sum up.
- This means that there is no phase relation between diffractions from different individuals.
- The measured intensities are the sum of the intensities from the individuals weighted by the volumes of the individuals.

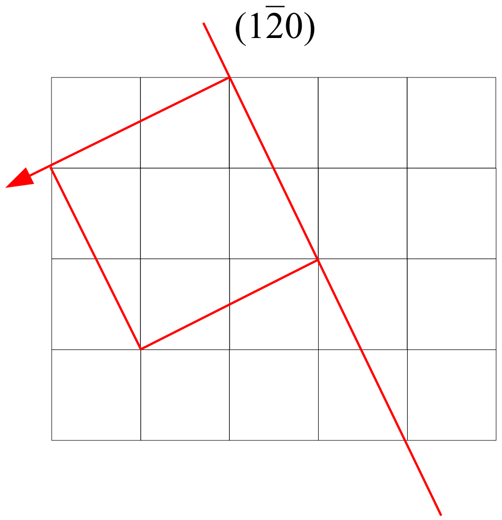
Problems related to twins. I. Effects of twinning on the diffraction pattern.



$$I_{obs} = V_1 I(h_1k_1l_1) + (1-V_1) I(h_2k_2l_2)$$

For n individuals: $I_{obs} = \Sigma_n V_n I(h_nk_nl_n)$

Example
$\{1\bar{2}0\}$ twin in melilite, $P\bar{4}2m$



Direction [*uvw*] perpendicular to a plane (*hkl*)

Crystal family	Lattice plane	Perpendicular direction
Triclinic	-----	-----
Monoclinic	(010)	[010]
Orthorhombic	(100), (010), (001)	[100], [010], [001]
Tetragonal	(*hk*0), (001)	[*hk*0], [001]
Hexagonal	(*hk*0), (001)	[2*h*+*k*, *h*+2*k*, 0], [001]
Cubic	(*hkl*)	[*hkl*]

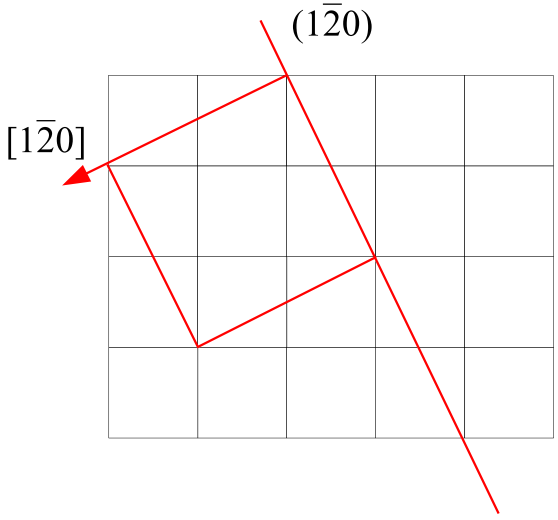
Directions [*uvw*] contained in a plane (*hkl*)

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 $hu+kv+lw = 0$.

{1$\bar{2}$0} twin in melilite ($P\bar{4}2m$)



$$\left(\boldsymbol{abc}\right)_I \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(\boldsymbol{abc}\right)_T$$

Miller indexes are covariant

$$\left(hkl\right)_I \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(hkl\right)_T$$

Representation of the twin operation in the twin basis

$$\begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Find non-equivalent reflections related by the twin operation

- Express the indexes of the reflections in the basis of the twin.
- Apply the twin operation in the basis of the twin and get the indices of the reflection related by twinning.
- Transform back the indices of this new reflection in the basis of the individual.

Effect of $\{1\bar{2}0\}$ twinning on $3\bar{1}1$ reflection

$3\bar{1}1$ Reflection from individual 1 in the setting of the twin

$$\left(3\,\bar{1}\,1\right)_I \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(551\right)_T$$

Reflection from individual 2

$$\left(551\right)_T \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(\bar{5}51\right)_T$$

Reflection from individual 2 in the setting of individual 1

$$\left(\bar{5}51\right)_T \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^{-1} = \left(\bar{5}51\right)_T \begin{bmatrix} 1/5 & \bar{2}/5 & 0 \\ 2/5 & 1/5 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(131\right)_I$$

$3\bar{1}1$ and 131 are not equivalent in $P\bar{4}2m$

$$\left(3\,\bar{1}\,1\right)\begin{bmatrix}0 & 1 & 0\\ \bar{1} & 0 & 0\\ 0 & 0 & 1\end{bmatrix} = \left(1\,3\,1\right)$$

Determinant = $+1$

Trace = $+1$

Symmetry operation = $4_{[001]}$

$$4_{[001]} \notin \bar{4}2m$$

Effect of $\{1\bar{2}0\}$ twinning on 100 reflection

Reflection from individual 1

$$(100)_I \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = (\ 120\ )_T$$

Reflection from individual 2

$$(120)_I \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = (\ \bar{1}20\ )_T$$

Reflection from individual 2 in the setting of individual 1

$$(\ \bar{1}20)_T \begin{bmatrix} 1 & 2 & 0 \\ \bar{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^{-1} = (\ \bar{1}20)_T \begin{bmatrix} 1/5 & \bar{2}/5 & 0 \\ 2/5 & 1/5 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left(\frac{3}{5}\, \frac{4}{5}\, 0 \right)_I$$

Non integers!

Effect of $\{1\bar{2}0\}$ twinning on 100 reflection

Norm of the vectors in reciprocal space

$$\sqrt{(100)\begin{bmatrix} 1/a^2 & 0 & 0 \\ 0 & 1/a^2 & 0 \\ 0 & 0 & 1/c^2 \end{bmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}} = 1/a$$

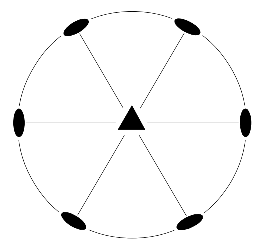
$$\sqrt{\left(\frac{3}{5}\,\frac{4}{5}\,0\right)\begin{bmatrix} 1/a^2 & 0 & 0 \\ 0 & 1/a^2 & 0 \\ 0 & 0 & 1/c^2 \end{bmatrix}\begin{pmatrix} 3/5 \\ 4/5 \\ 0 \end{pmatrix}} = 1/a$$

Effect of $\{1\bar{2}0\}$ twinning on 100 reflection

A reflection from individual **1** is repeated by the twin operation in a position where there is no reflection from the individual **2**. If the second position is not rational (non-integer indexes) the software will not find the unit cell of the individual, but only that of the twin, without knowing it is a twin.
If the second position is rational but correspond to an absent reflection from individual 2, then the systematic absences are affected and you won't get the right space group.
If the second position correspond to a present reflection from individual 2, then the measure intensity is the sum (***not*** interference!) of the intensities from the two individuals.
In any case, you won't be able to refine the structure unless you into account the presence of twinning.

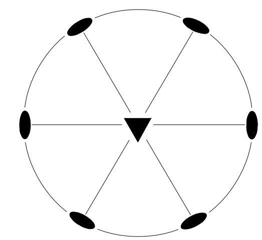
Problems related to twins. II. Effects of twinning on physical properties.

Swiss twin in α quartz

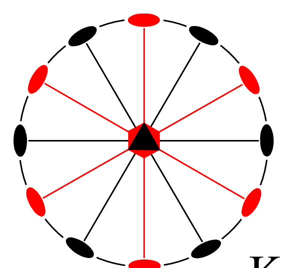


K = 321 (D_3)

$\hat{t} = 2_{[001]}$



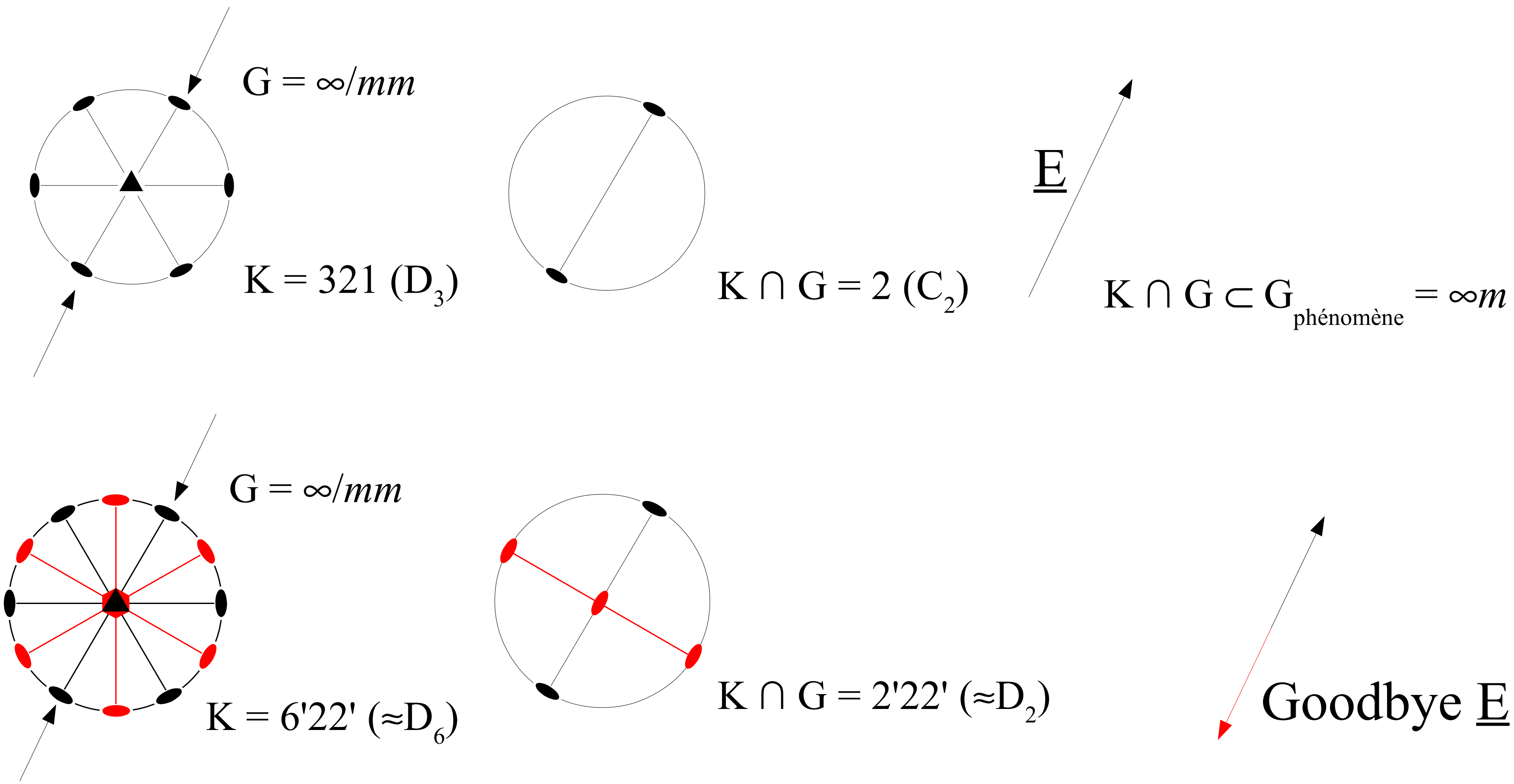
K = 321 (D_3)



K = 6'22' ($\approx D_6$)

Killing of piezoelectricity

Interpretation of piezoelectricity in α quartz by Curie law

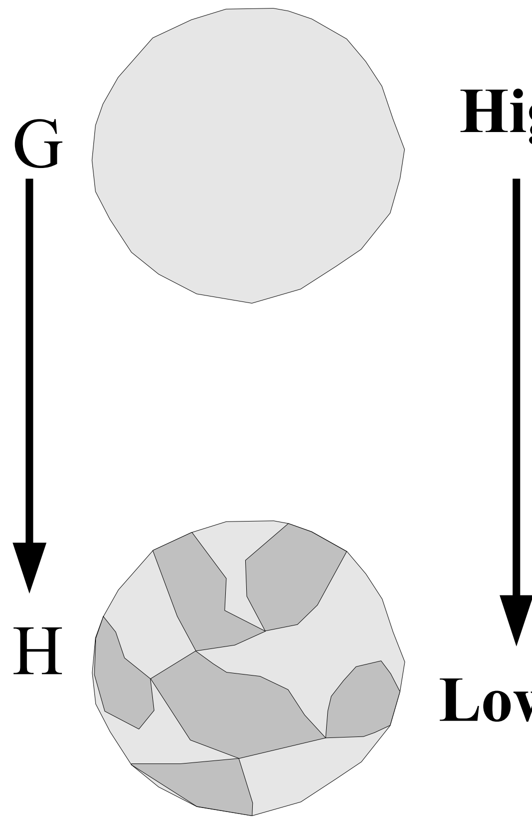


Genetic classification of twins - 1

Transformation twins. Driving force: symmetry change following a phase transition

High-symmetry (parent) phase

Group-subgroup relation (translationengleiche)

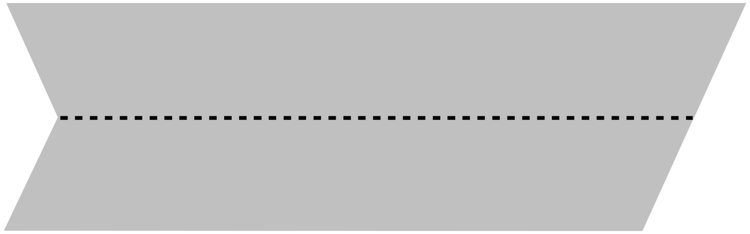


$i_p = |G| / |H|$ = No. of domain states

Low-symmetry (daughter) phase

Genetic classification of twins - 2

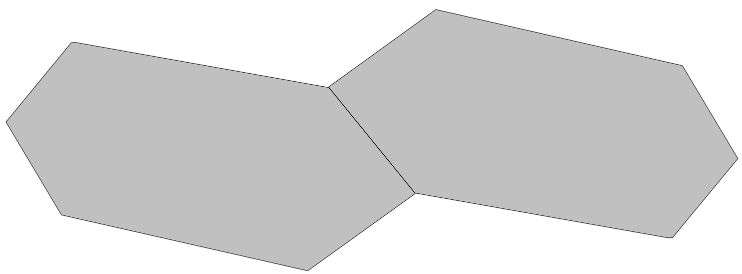
Mechanical twins. Driving force: the application of an external force



In general, no precise symmetry relation between the original crystal and the resulting twin.

Genetic classification of twins - 3

Growth twins. Driving force: the "randomness" (errors in crystal growth or coalescence of nano or macrocrystals)



No symmetry relation between the original crystal and the resulting twin.

For the formation of the twin, the of the interface is important: a substructure must continue, precisely or approximately, across the interface.

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, centre) 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.

Example of twin law *vs*. twin operation & twin element

Crystal belonging to the geometric crystal class 2 (*b*-unique) twinned by 120º about [001]

$$\{1, 2_{[010]}\} \cup \{3^{+}_{[001]}, 2_{[110]}\} \cup \{3^{-}_{[001]}, 2_{[100]}\}$$

Two twin laws: the two cosets $\{3^{+}_{[001]}, 2_{[110]}\}$ and $\{3^{-}_{[001]}, 2_{[100]}\}$

Four twin operations – the four operations in the two cosets

Three twin elements: [001], [110] and [100]

Symmetry of the twin expressed by a trichromatic point group (twin point group): $(3^{(3)}2^{(2,1)})^{(3)}$

The twin lattice is hexagonal

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

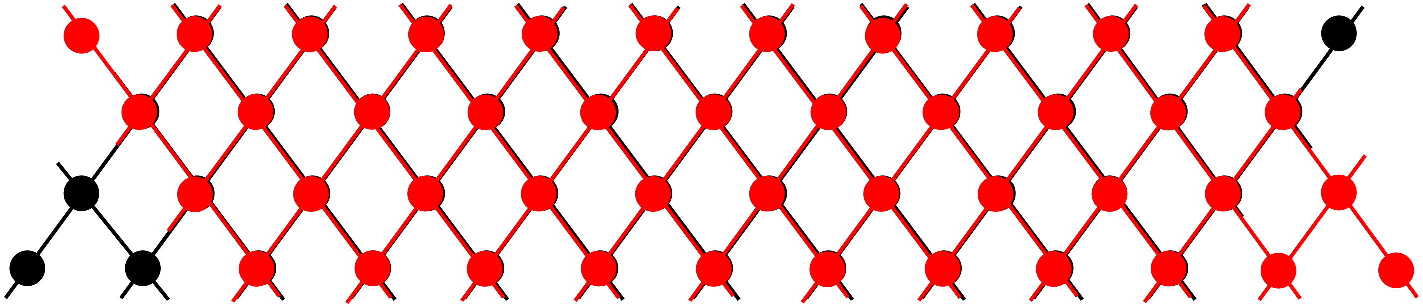
- The twin index is the number of lattice nodes restored or quasi-restored by the twin operation.
- The (quasi)-restored nodes define a lattice, the **twin lattice**.
- (Quasi)-restored nodes define the cell based on the pair of elements (plane/direction) defining the cell of the twin lattice.
- The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

Reticular classification of twins

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



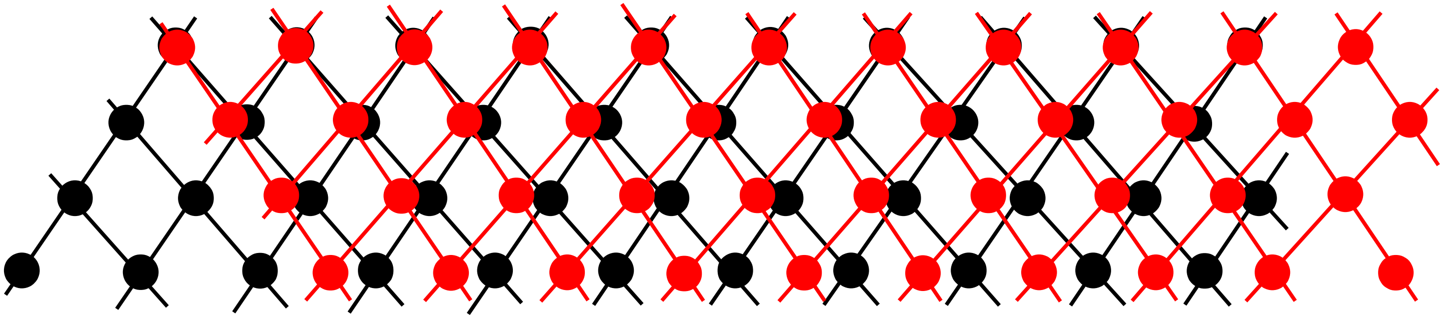
All nodes are restored by the twin operation: we say that **the twin index is *n* = 1**

$$H^* = H;\ K \supset H$$

Subclassification 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**

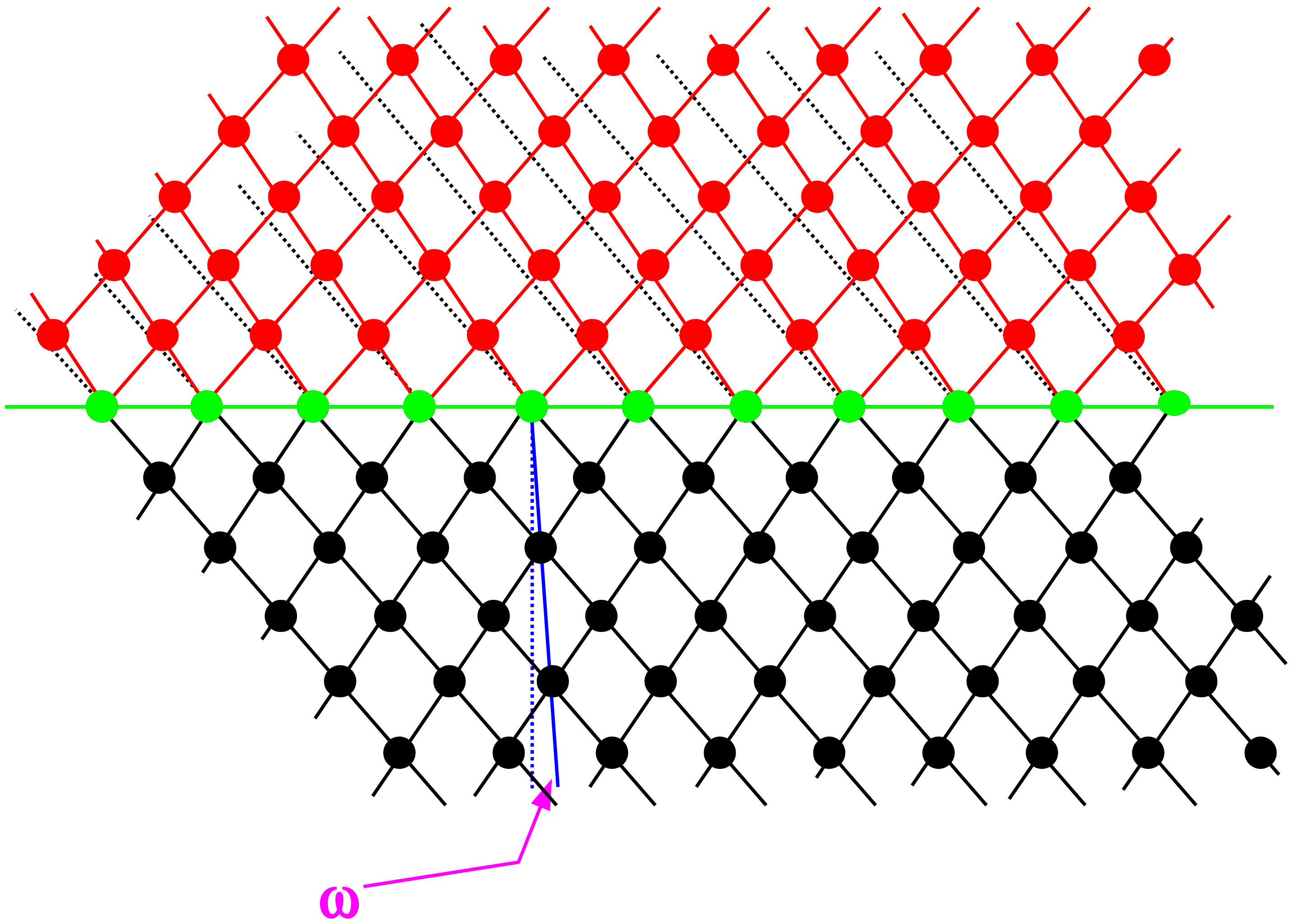
Twinning by pseudo-merohedry



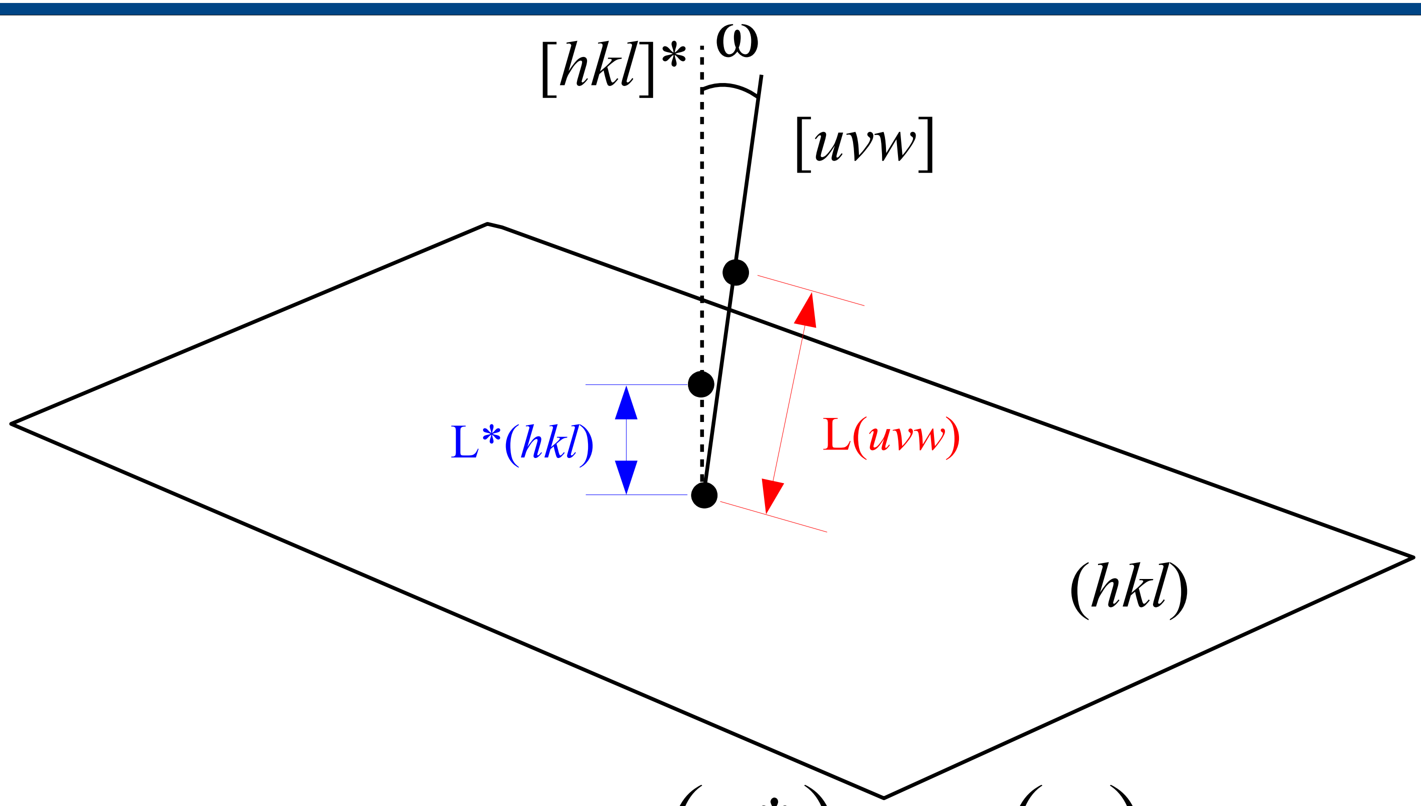
All nodes are *quasi*-restored by the twin operation: we say that **the twin index is *n* = 1**

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

Definition of obliquity



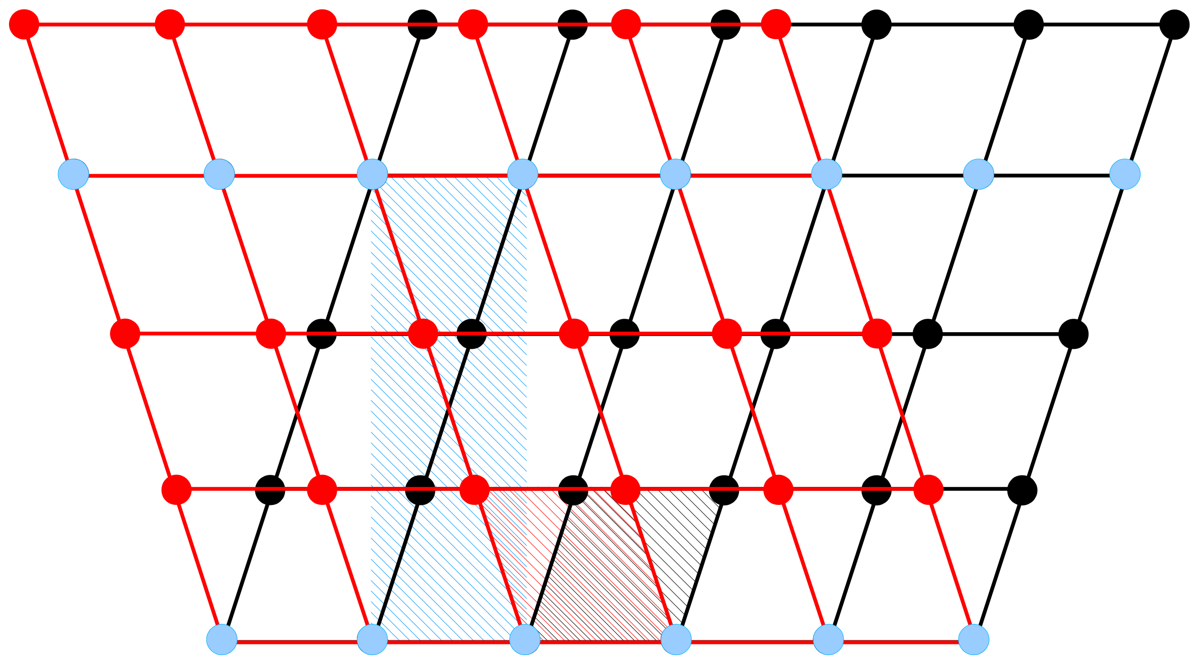
Computation of the obliquity



$$L^*(hkl)L(uvw)\cos\omega = \begin{pmatrix} h & k & l \end{pmatrix} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} \begin{pmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = |hu+kv+lw|$$

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

Twinning by reticular merohedry

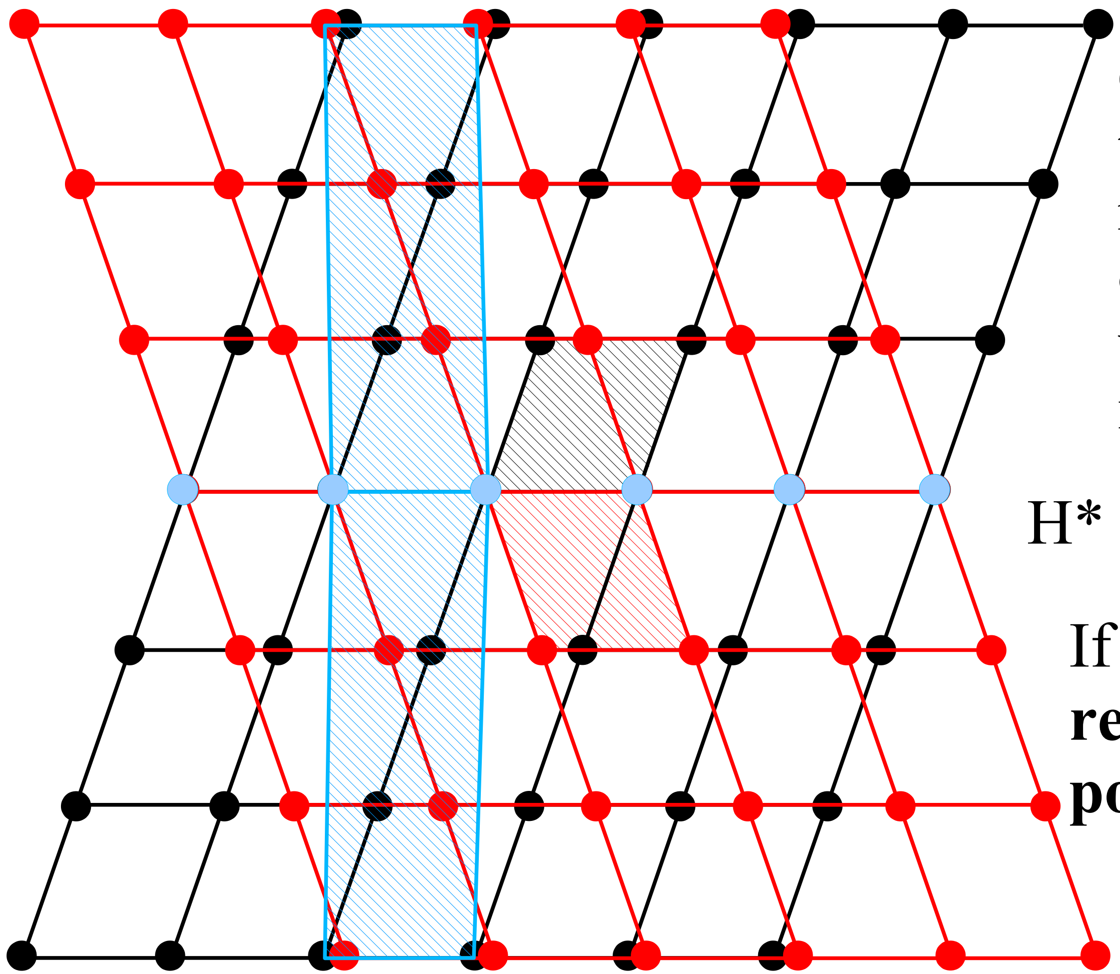


One node out of three is restored by the twin operation: we say that **the twin index is *n* = 3**

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 $\boldsymbol{n}$ = 3**

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

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

A note of nomenclature

"Merohedral" vs. "merohedric"

$H = 2$, $\beta \neq 90^\circ$ — The individual is ***merohedral*** (the holohedral point group being 2/*m*)

Inversion twinning: $K = 2/m'$ — Twinning by merohedry, or **merohedric** (**NOT** *merohedral*) twinning.

$H = 2$, $\beta \approx 90^\circ$ — The individual is still ***merohedral***

Rotation twinning: $K = 2'22'$

Reflection twinning: $K = m'2m'$

Twinning by pseudo-merohedry, more generally **non-merohedric** (**NOT** *non-merohedral*) twinning.

Why a *reticular* theory of twinning?

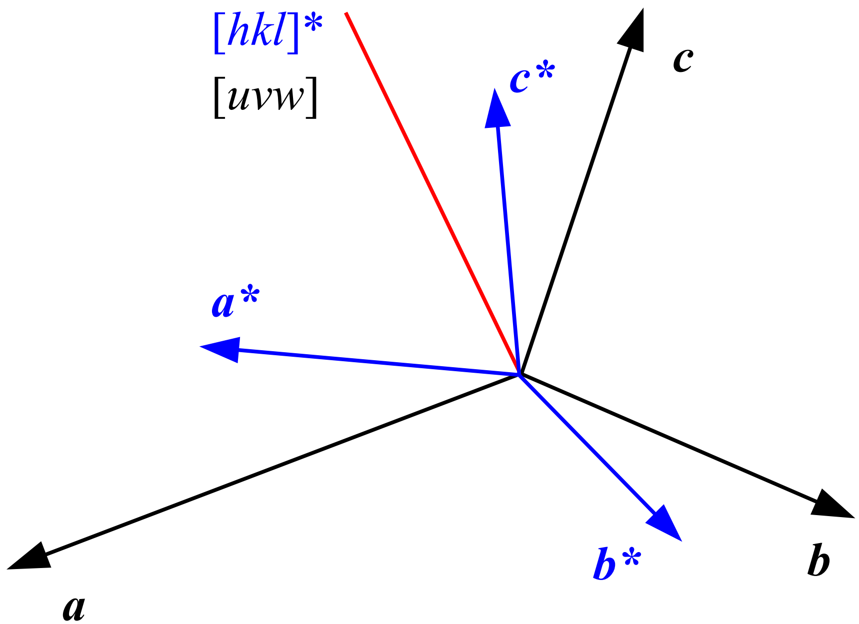
- Twinning is governed by the structural match at the interface of the individuals.
- To study this structural match means to investigate twins *case by case*.
- The reticular theory makes abstraction of the structure and concentrates on the lattice.
- This approach is reasonable, although approximate, because the lattice represents the periodicity of the structure.
- A good lattice match is a necessary, although not sufficient, condition for a good structural match.

Probability occurrence of twins in term of the reticular theory

- A twin is a "mistake" or a "compromise".
- A coherent or semi-coherent interface is necessary for a twin to form.
- The better is the "atomic restoration" the higher is the probability that a twin occurs.
- The analysis of the atomic restoration reduces the study of twins almost to a "case-by-case" investigation.
- The reticular theory allows a general approach in terms of lattice restoration as a necessary (not sufficient) condition.
- The lower are the twin index and the obliquity, the higher is the probability that a twin occurs.

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:

$$\left(hkl\right)\begin{pmatrix}\boldsymbol{a}^*\\ \boldsymbol{b}^*\\ \boldsymbol{c}^*\end{pmatrix}=\left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}\qquad \left(hkl\right)\mathbf{I}\begin{pmatrix}\boldsymbol{a}^*\\ \boldsymbol{b}^*\\ \boldsymbol{c}^*\end{pmatrix}=\left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}$$

$$\left(hkl\right)\mathbf{G}^*\mathbf{G}\begin{pmatrix}\boldsymbol{a}^*\\ \boldsymbol{b}^*\\ \boldsymbol{c}^*\end{pmatrix}=\left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}$$

$$\left(hkl\right)\mathbf{G}^*\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}\left(\boldsymbol{abc}\right)\begin{pmatrix}\boldsymbol{a}^*\\ \boldsymbol{b}^*\\ \boldsymbol{c}^*\end{pmatrix}=\left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}$$

$$\boldsymbol{v}_{\mathrm{i}}\cdot\boldsymbol{v}_{\mathrm{j}}^* = \delta_{\mathrm{ij}}$$

Easy!

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

$$\left(hkl\right)\mathbf{G}^*\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix} = \left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}$$

$$\left(hkl\right)\mathbf{G}^* = \left(uvw\right)$$

and of course... $\left(uvw\right)\mathbf{G} = \left(hkl\right)$

Exercise

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

Twinned on (210)

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

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

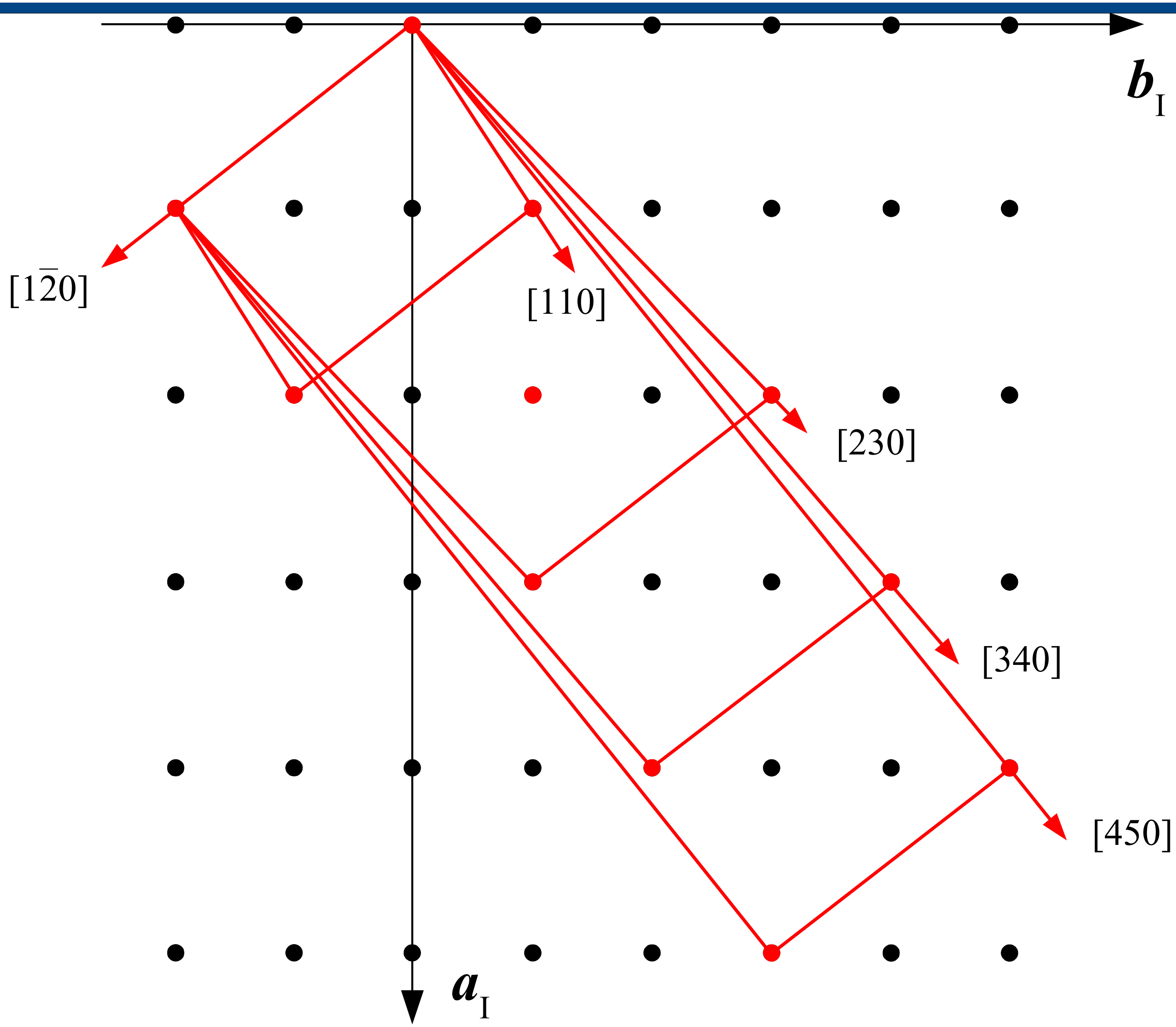
u	***v***	***v/u***
1	1	1
1	2	2
2	3	1.5
3	4	1.333
4	5	1.25

Calculate the obliquity

$$\omega = \cos^{-1}|hu+kv+lw|/L^*(hkl)L(uvw) = \cos^{-1}\frac{\left|\left(hkl\right)\begin{pmatrix}u\\v\\w\end{pmatrix}\right|}{\sqrt{\left(hkl\right)\mathbf{G}^*\begin{pmatrix}h\\k\\l\end{pmatrix}}\sqrt{\left(uvw\right)\mathbf{G}\begin{pmatrix}u\\v\\w\end{pmatrix}}}$$

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

Exercise: results



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

Summary

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

Smaller index, larger obliquity

Smaller obliquity, larger index

Which one would you choose? **Both!**

(210) twin in celestine is a hybrid twin

How many lattice nodes in the cell of $\mathbf{L}_T$?

10

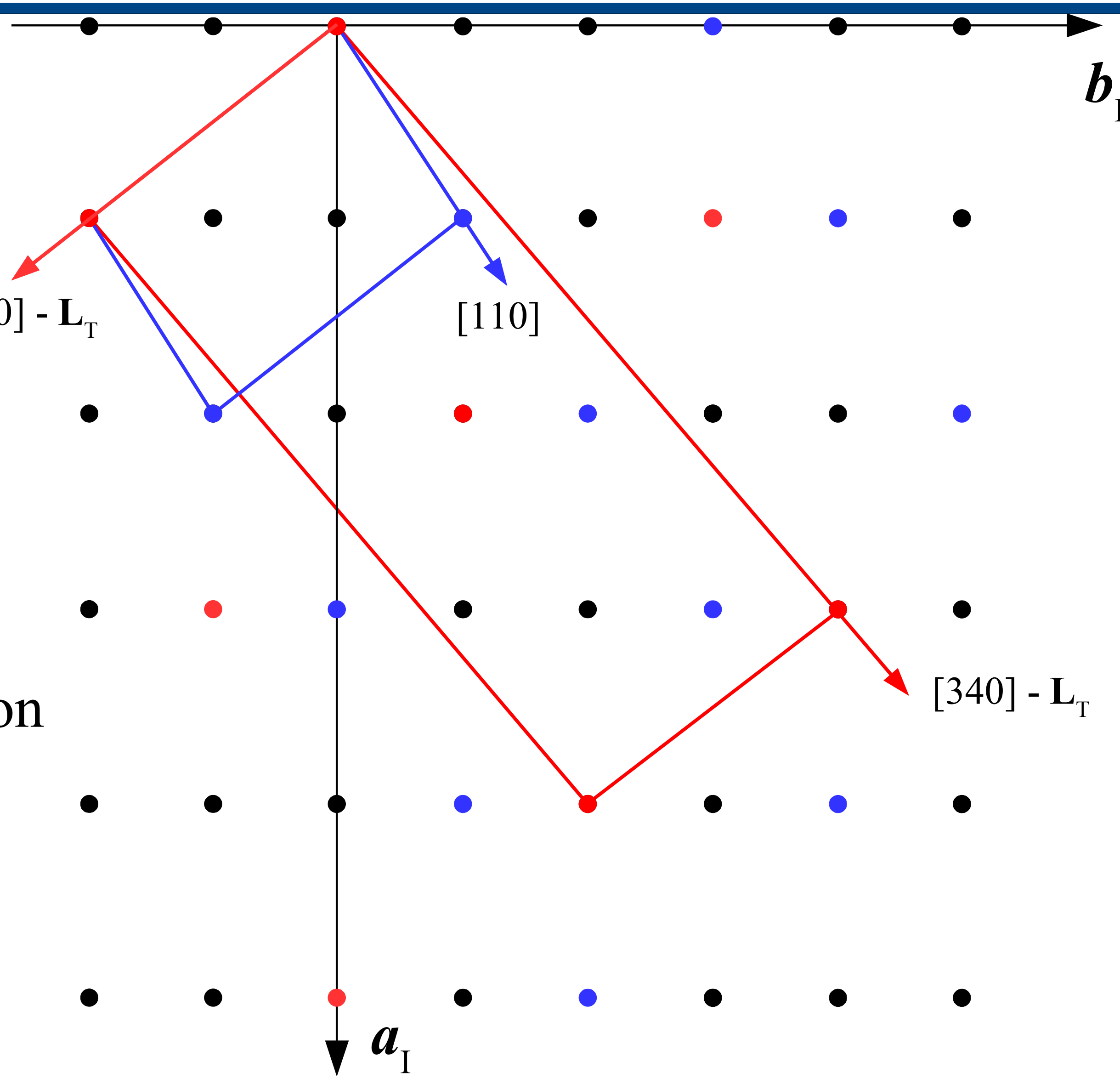
How many of these belong to the red or blue sublattice?

5

Global lattice restoration due to twinning?

10/5 = 2.0

Effective twin index



Cell parameters of the twin lattice

A matter of basis transformation....

$$(\boldsymbol{a} \quad \boldsymbol{b} \quad \boldsymbol{c})\,\mathbf{P} = (\boldsymbol{a}' \quad \boldsymbol{b}' \quad \boldsymbol{c}')$$

$$\mathbf{G}' = \begin{pmatrix} \boldsymbol{a}' \\ \boldsymbol{b}' \\ \boldsymbol{c}' \end{pmatrix} (\boldsymbol{a}' \quad \boldsymbol{b}' \quad \boldsymbol{c}') = \mathbf{P}^t \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{pmatrix} (\boldsymbol{a} \quad \boldsymbol{b} \quad \boldsymbol{c})\,\mathbf{P} = \mathbf{P}^t\mathbf{G}\mathbf{P}$$

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

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*)

Cell parameters of the (210) twin in celestine based on (210)/[340] cell

$$[u_{1,hkl}v_{1,hkl}w_{1,hkl}] = [001]$$

$$[u_{2,hkl}v_{2,hkl}w_{2,hkl}]\ [1\bar{2}0]$$

$$[u_{\perp}v_{\perp}w_{\perp}]=[340]$$

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

$$|\mathbf{P}| = 10 > 0$$

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

Cell parameters of the (210) twin in celestine

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

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

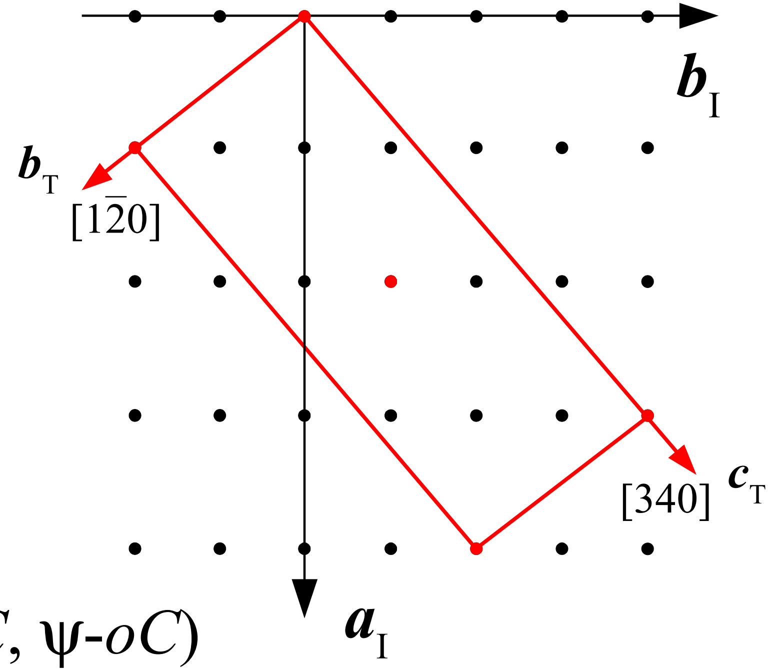
$$a_\mathrm{T} = c_\mathrm{I} = 6.866 \text{ Å} \qquad b_\mathrm{T} = 13.581 \text{ Å} \qquad c_\mathrm{T} = 32.972 \text{ Å}$$

$$\alpha_\mathrm{T} = \cos^{-1}\frac{3a^2 - 8b^2}{b_\mathrm{T}c_\mathrm{T}} = \cos^{-1}\frac{-19.533}{13.581 \cdot 32.972} =$$

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

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

Now that you know how to do it, let a software do it for you....

CRM2 ▾ RECHERCHE ▾ FORMATION ▾ SERVICES ▾ LOGICIELS ▾ PUBLICATIONS RECHERCHE

Geminography

Geminography

Auteur : Massimo NESPOLO

Publications :

M. Nespolo, G. Ferraris (2006). The derivation of twin laws in non-merohedric twins – Application to the analysis of hybrid twins. Acta Crystallogr. A62, 336-349. Electronic reprint (330 Kb)

Le logiciel **geminography** explore les possibles lois de macles. Il prend en input les paramètres de maille et les indices de l'élément de macle (connu ou soupçonné), plus d'autres paramètres décrits dans la documentation, et explore les éléments du réseau (quasi)-perpendiculaires pour repérer les possibles sous-réseaux. Il calcule l'indice de macle et l'obliquité, ainsi que la pseudo-symétrie des sous-réseaux. Ce logiciel effectue une recherche systématique des sous-réseaux coexistants et décrit les macles comme hybrides chaque fois que cette description rend compte de la quasi- superposition réticulaire mieux que la description classique, qui utilise au contraire un seul sous-réseau.

Plus de détails : http://www.crystallography.fr/pages_perso/Nespolo/en/geminography.php

Fichier exécutable (MS-DOS/Windows) : geminography.zip

News

Conférence Dr. Luigi Paolasini
Le Dr. Luigi Paolasini, de l'ESRF Grenoble, donnera une conférence le Mercredi 9 avril à 10h00 dans la salle de conférence du laboratoire CRM2 (niveau 3 entrée 3B) intitulée : « Magnetic elastic diffraction by hard x-rays ». Abstract

Conférence Dr. Lebègue
Le jeudi 10 avril à 14h30 en Salle Jean Barriol, Faculté des Sciences et Technologies, Entrée 2A, Niveau 7, Le Dr. Sébastien Lebègue Equipe Modélisation Quantique, CRM2, CNRS-Université de Lorraine. Donnera une conférence intitulée : « New two dimensional compounds : beyond carbon and beyond graphene. » Résumé In the field of nanosciences, the quest for mate [...]

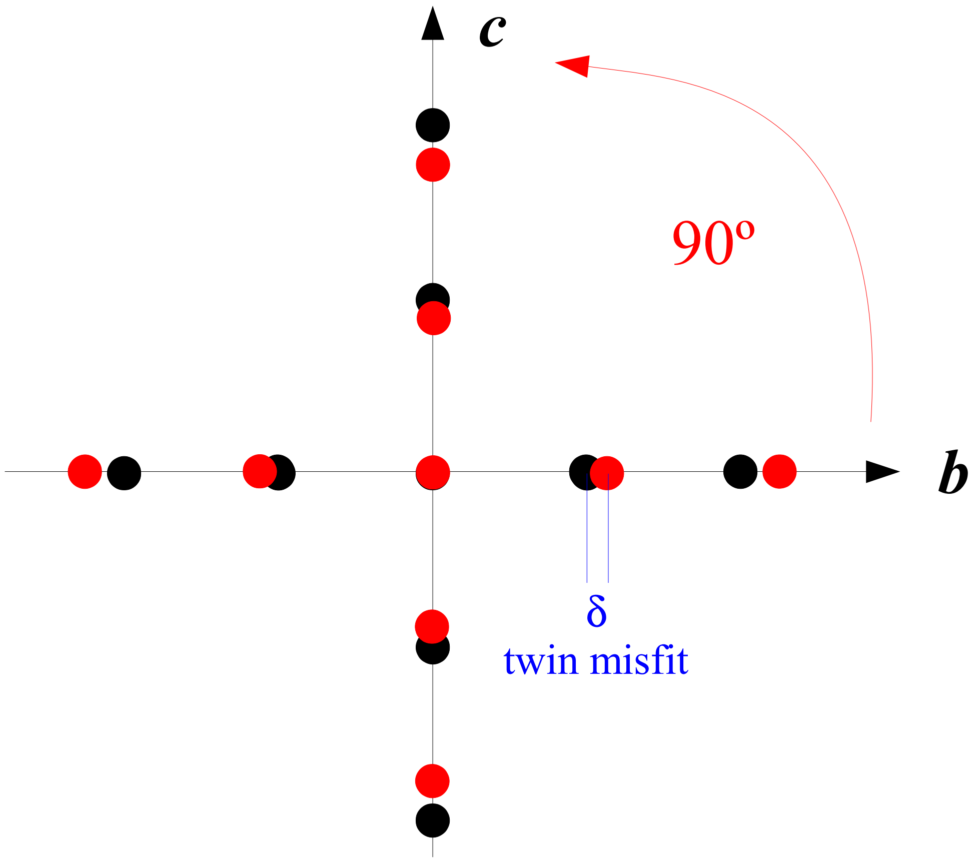
http://www.crystallography.fr/lab/geminography/

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

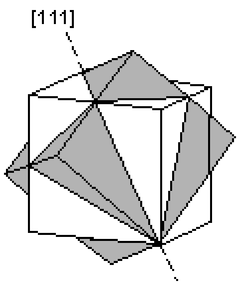
$b \approx c$



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)	(001) (*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(°)	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

To read more and find references...

International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

Research themes: Crystal twinning

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http://www.crystallography.fr/mathcryst/twins.htm

Contributed by Massimo Nespolo

Last update: 3 February 2009

This page is optimized for a 1024 x 768 screen resolution and uses javascript pop-up windows. To see them, you need a javascript-enabled browser. If you use a pop-up stopper, set it to accept on-request pop-up.
This page follows the W3C standards. Nevertheless, some tags and characters (ex. the negative indices) are not correctly shown by Internet Explorer. We recommend browsing with Opera (Mozilla / Firefox may work too).

The study of twinned crystals can be traced back to the early morphological observations (Steno, 1669). Nowadays, twinned crystals are often considered an obstacle to automatic solution and refinement of crystal structures. As a matter of fact, the study of twins in itself developed, thanks to several prominent crystallographers especially between the XIX and the XX centuries, almost as a specialistic branch inside crystallography. For this reason, J.D.H. Donnay introduced the term **geminography** to specifically indicate this branch of crystallography (historical note).