Domain structures and twinning

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Massimo Nespolo, Université de Lorraine, France
massimo.nespolo@univ-lorraine.fr

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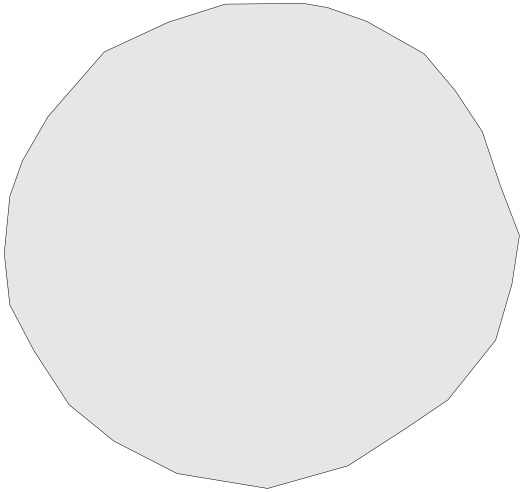
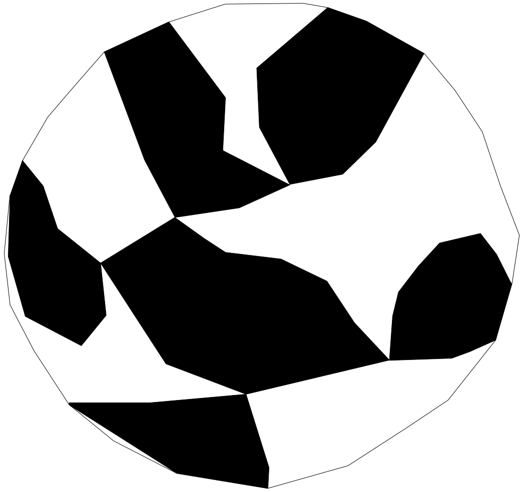
Basic definitions

Domain structures

Domain structures are heterogeneous structures composed of homogeneous regions, called (you guess it!)…. domains!



A homogeneous structure



A heterogeneous structure composed of two domain states (variants), occurring as N domains physically separated in space

Isomorphic substitution and substitutional disorder

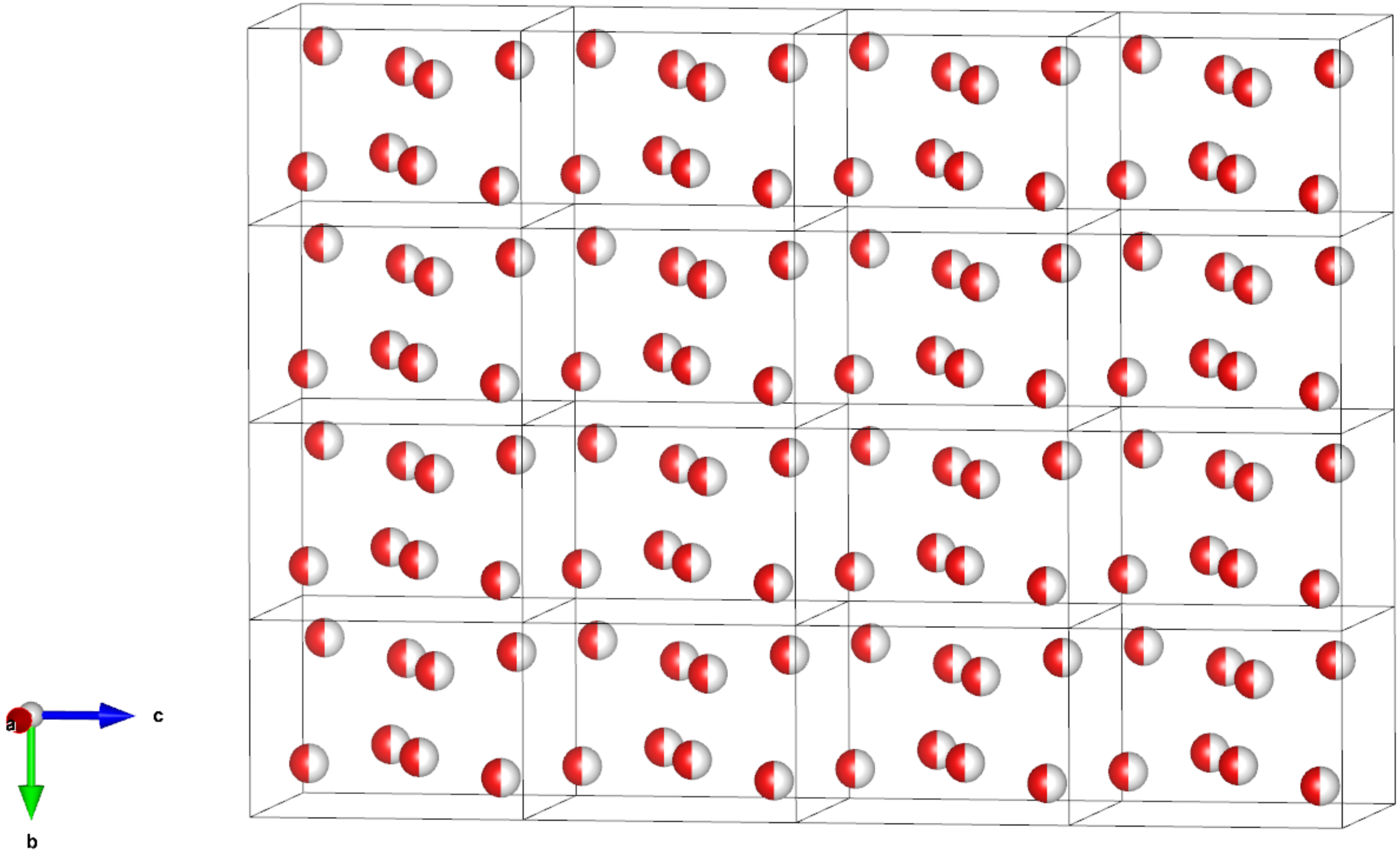


figure drawn with VESTA (http://jp-minerals.org/vesta/en/)

Isomorphic substitution and substitutional disorder

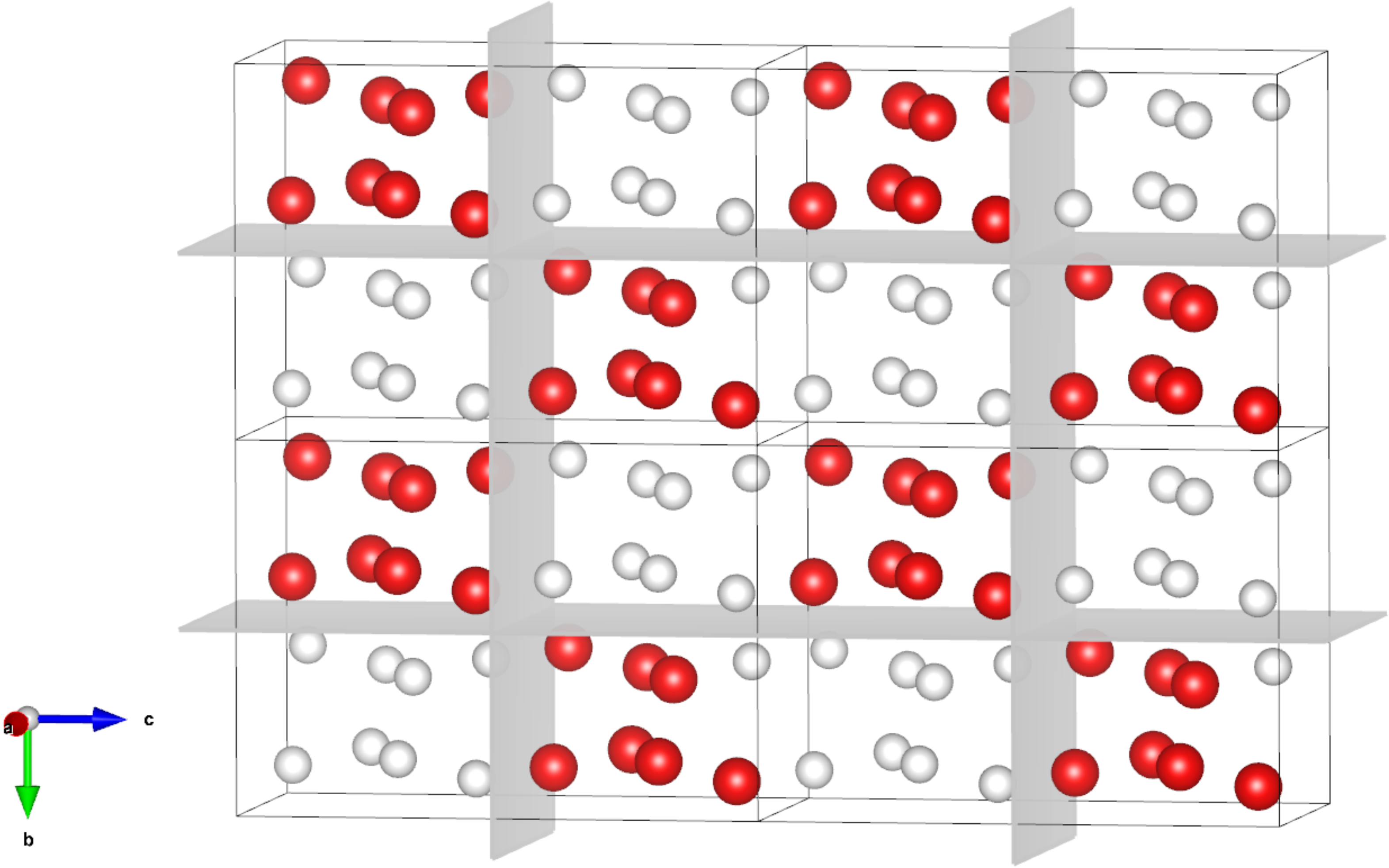


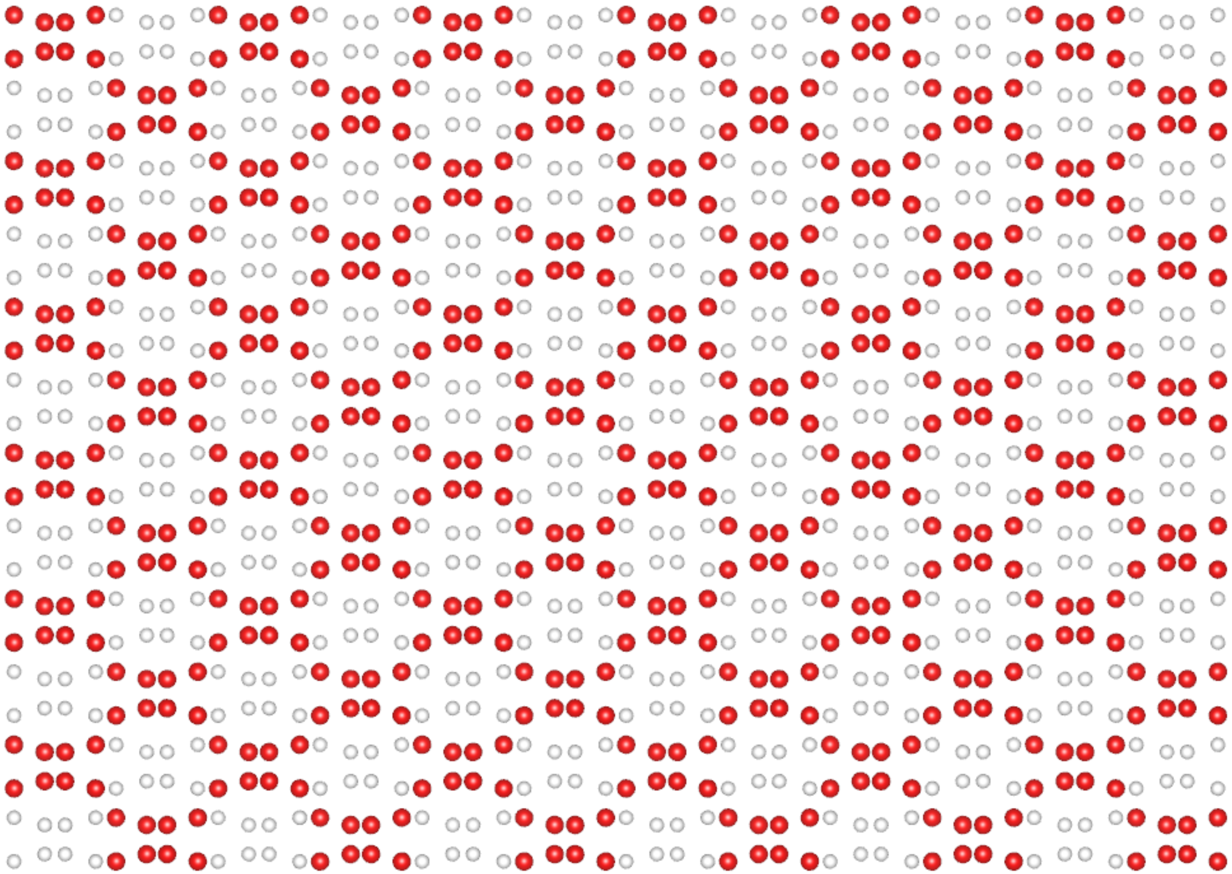
figure drawn with VESTA (http://jp-minerals.org/vesta/en/)

Types of domain states

Depending on the type of heterogeneity, domain states can be classified as follows:

- **chemical domains**: the domain states differ for their chemical composition;
- **ferroelectric domains**: the domain states differ for the direction of the polarization vector;
- **magnetic domains**: the domain states differ for the orientation of the magnetic dipole moments;
- **translation domains**: the domain states differ for their relative position, not related by a translation vector of the structure;
- **orientation domains**: the domain states differ for their relative orientation, not related by a (proper or improper) rotation operation of the structure.

Antiphase domains



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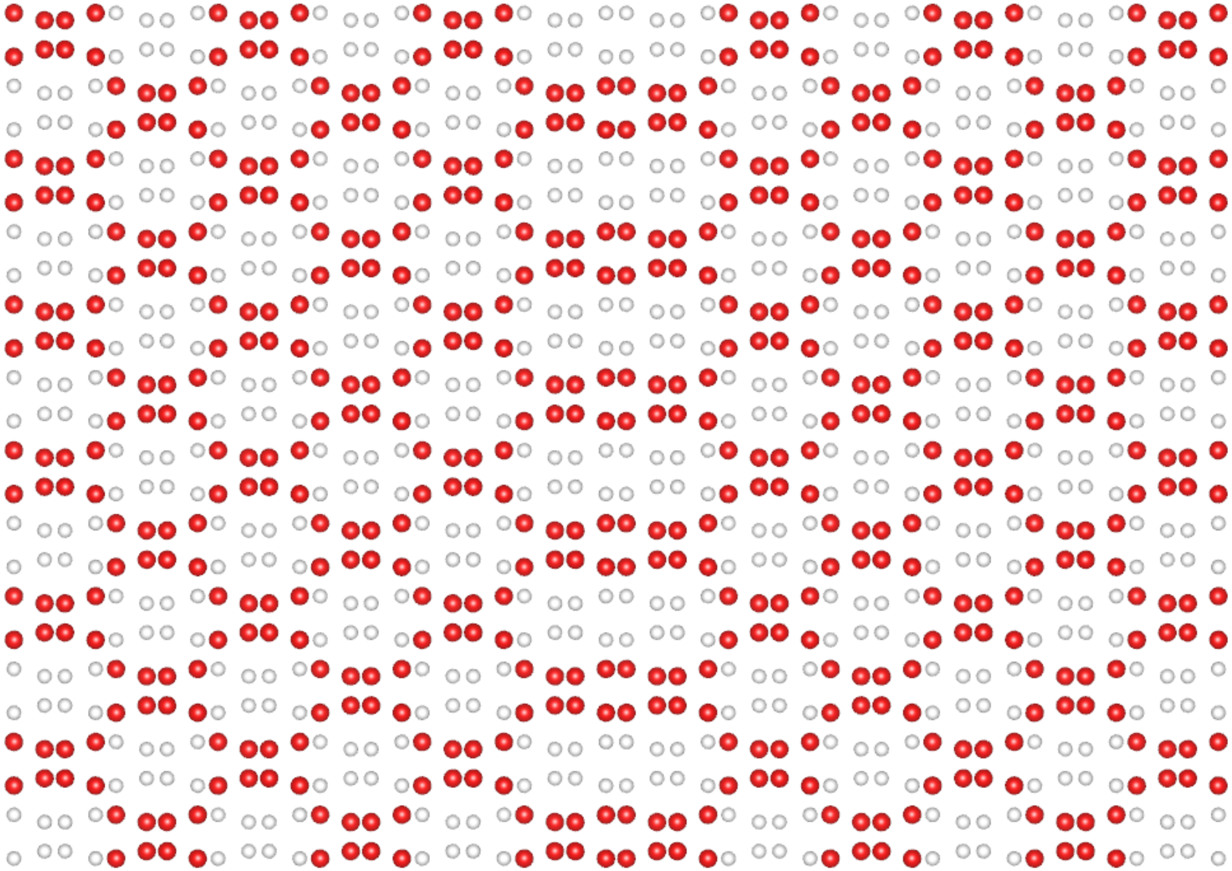
Antiphase domains



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Antiphase domains

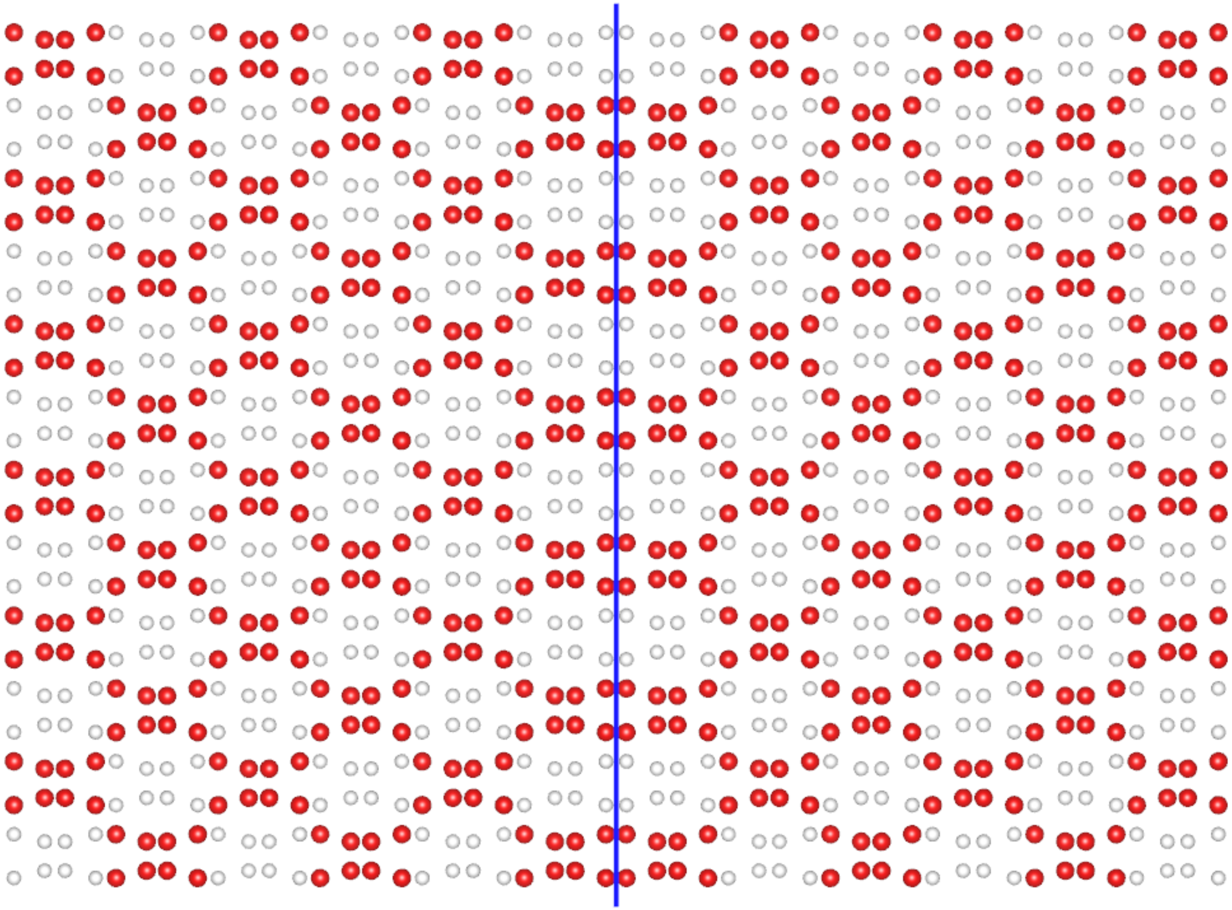
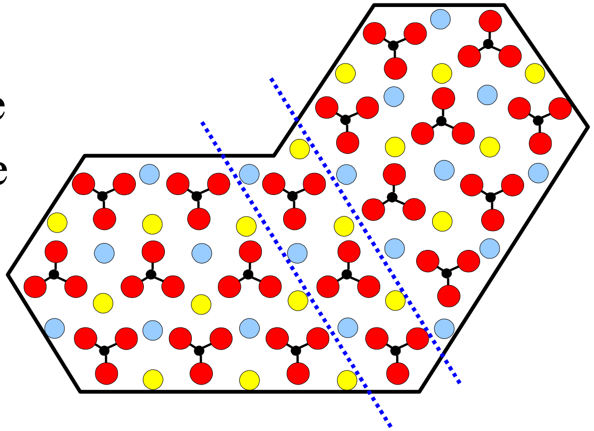


figure drawn with VESTA (http://jp-minerals.org/vesta/en/)

Twin domains

The operation mapping the **orientation** of one domain state onto that of another domain state is a **crystallographic** operation not belonging to the point groups of the domains

- ● Oxygen
- • Carbon
- ● Ca above the CO_3 plane
- ● Ca below the CO_3 plane



Aragonite, $CaCO_3$, twinned on (110)

H_i = point group of the i-th domain state D_i

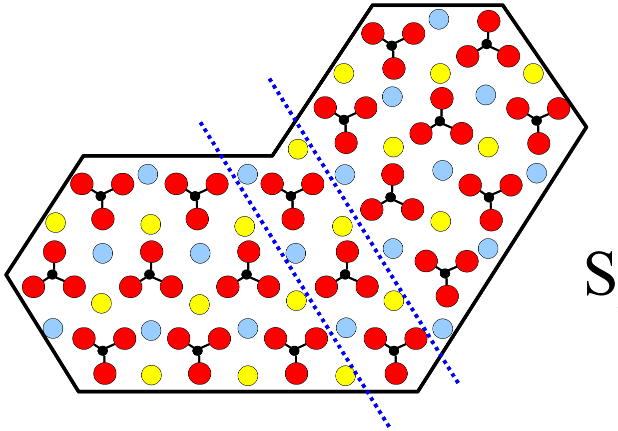
φ_i = operation mapping $D_1 \rightarrow D_i$

$$H_i = \varphi_i H_1 \varphi_i^{-1}$$

Twin domains (cont.)

Domain D_1

Space group G_1



Domain D_2

Space group G_2

G_1 and G_2 are of the **same type** (same Hermann-Mauguin symbol) but are **different groups** because corresponding symmetry elements are **differently oriented in space**.

$tD_1 = D_2$ $\quad D_1 = t^{-1}D_2$ $\quad t(g_{1,i}D_1) = g_{2,j}D_2$ $\quad tg_{1,i}t^{-1}D_2 = g_{2,j}D_2$

$g_{2,j} = tg_{1,i}t^{-1}, \forall i,j$

$G_2 = tG_1t^{-1}$

conjugation

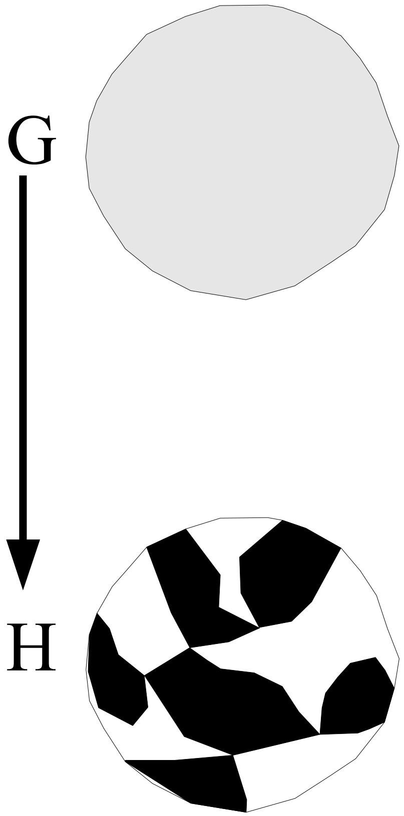
(a similarity transformation)

How do domains form?

Genetic classification of domains

1 – Transformation domains

Origin: symmetry change under a phase transition



Group-subgroup relation

High-symmetry (parent) phase

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

$i = i_P i_L$, i_P = index of the point group, i_L = index of the sublattice

i_P = number of twin domain states

i_L = number of antiphase domain states

Low-symmetry (daughter) phase

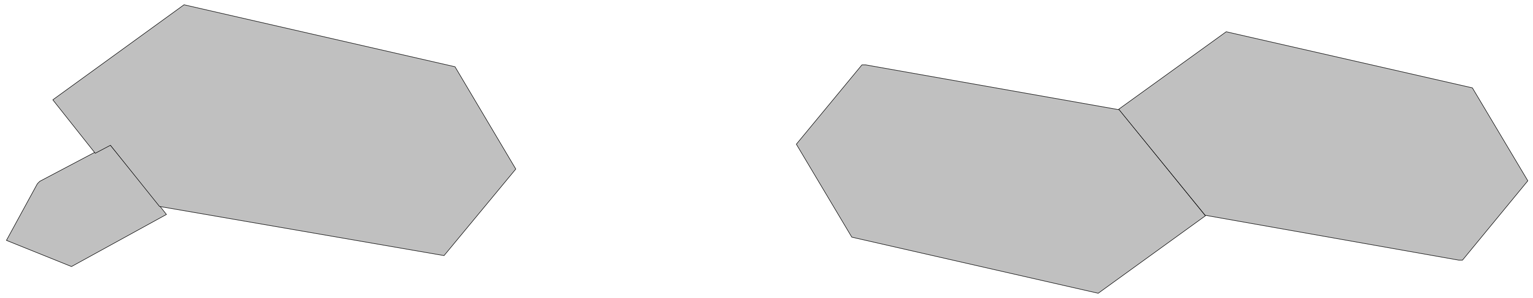
2 – Mechanical domains

Origin: the application of an external force

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

3 – Growth domains

Origin: the “randomness” (errors in crystal growth or coalescence of nano, micro or macrocrystals*)



No *a-priori* symmetry relation between the original crystal and the resulting domain structure.

* http://dx.doi.org/10.1127/0935-1221/2004/0016-0401

Classification of subgroups (reminder)

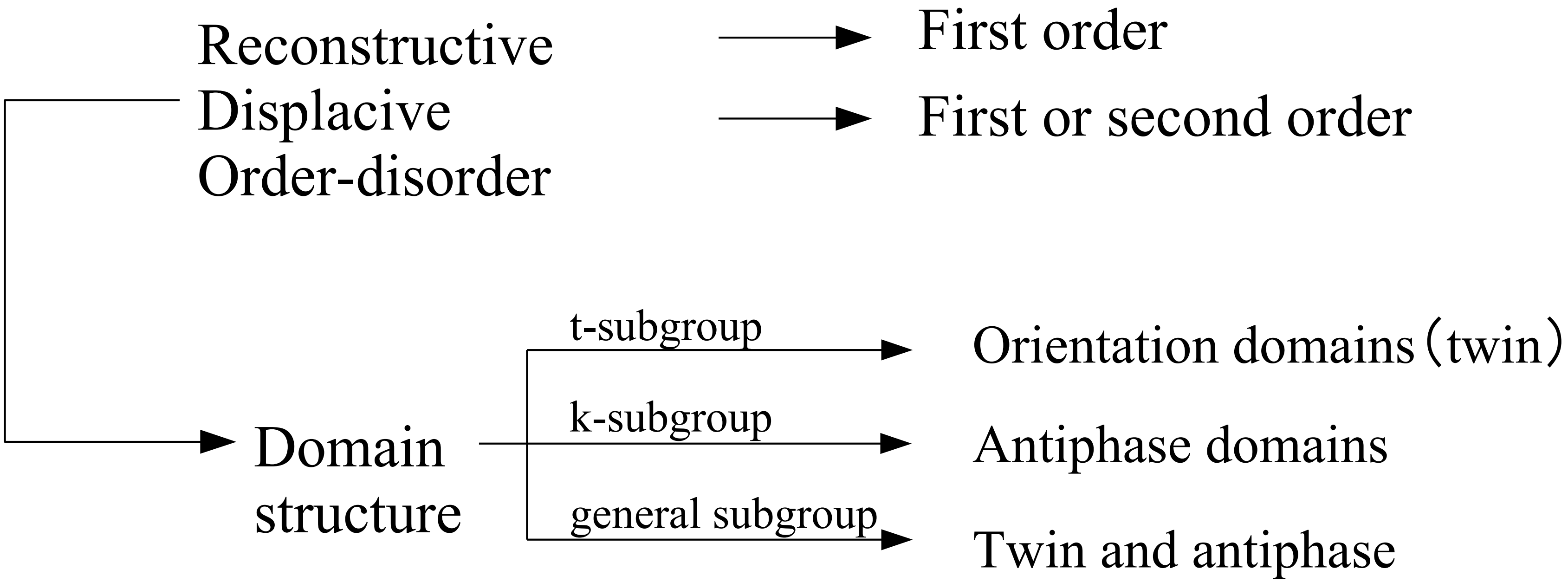
- G and {1} are the **trivial subgroups** of G.
- All the other subgroups are called **proper subgroups**.
- Let it be G ⊃ H. If there is not group intermediate between H and G, then H is called a **maximal subgroup** of G.
- If G and H has all the translations in common, then H is called a **translationengleiche subgroup** (t-subgroup) of G.
- IF G and H belong to the same geometric crystal class (have the same point group), then H is called a **klassengleiche subgroup** (k-subgroup) of G.
- Let H be a k-subgroup of G. If G and H belong to the same space-group type (they have the same Hermann-Mauguin symbol), then H is called an **isomorphic subgroup** (i-subgroup) of G.

Reduction of symmetry following a phase transition

Thermodynamic classification of phase transitions (Ehrenfest and Tisza)

First order, second order, lambda....

Buerger’s classification



Reconstructive → First order

Displacive → First or second order

Order-disorder

Domain structure

t-subgroup → Orientation domains（twin）

k-subgroup → Antiphase domains

general subgroup → Twin and antiphase

Index： Number of (types of) domains Cosets: Orientation and position of domains

Exercise

$SrTiO_3$, perovskite structure type, space-group type $Pm\bar{3}m$

Low-temperature phase (below 105K): octahedra rotation produces lowering of symmetry

$$Pm\bar{3}m \rightarrow I4/mcm$$

$$c \rightarrow 2c$$

V → 4V (V: volume of the unit cell)

Following this phase transition:

Determine the number of twin domain states

Determine the number of antiphase domain states

Determine the operation (coset representative) that maps each pair of domain state

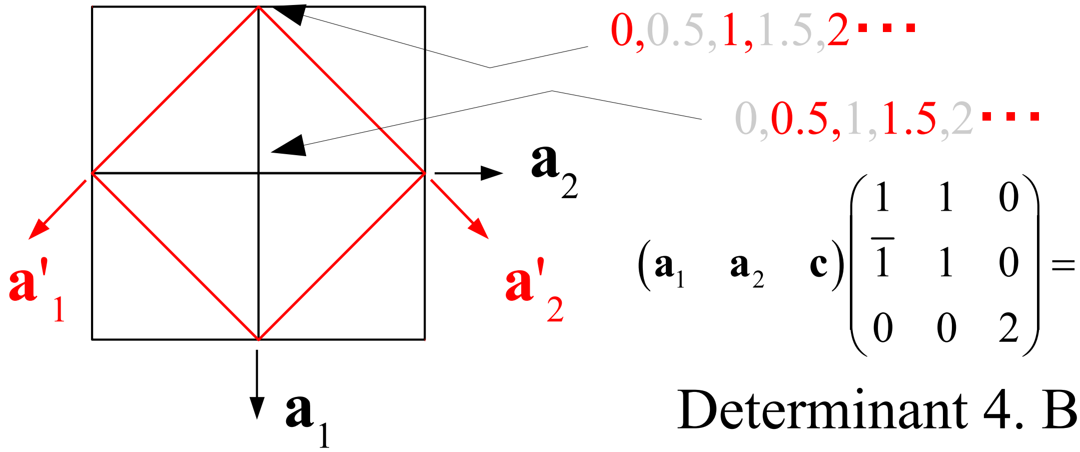
Exercise (solution)

$Pm\bar{3}m \rightarrow I4/mcm$

$c \rightarrow 2c$

$V \rightarrow 4V$

$z = 0,1,2,3,4 \cdots \rightarrow 0,0.5,1,1.5,2 \cdots$



$$\begin{pmatrix}\mathbf{a}_1 & \mathbf{a}_2 & \mathbf{c}\end{pmatrix}\begin{pmatrix}1 & 1 & 0\\ \bar{1} & 1 & 0\\ 0 & 0 & 2\end{pmatrix} = \begin{pmatrix}\mathbf{a}'_1 & \mathbf{a}'_2 & \mathbf{c}'\end{pmatrix}$$

Determinant 4. BUT $P \rightarrow I$

$i_L = 2$

$i_P = |m\bar{3}m|/|4/mmm| = 48/16 = 3$

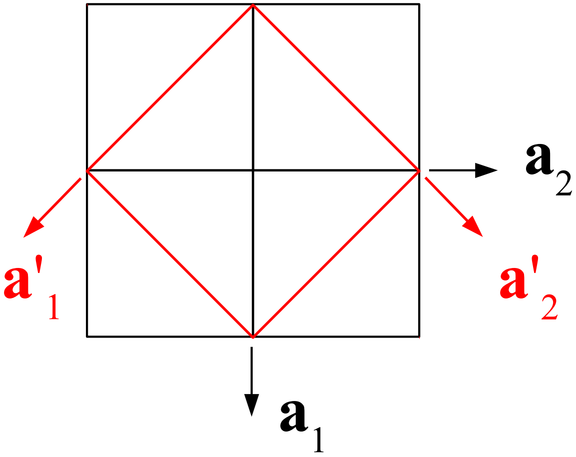
$i = i_P \cdot i_L = 3 \cdot 2 = 6$

6 types of domain states. Taking one as reference:

- 3 pairs are in twin relation (one trivial)
- the other 3 are in antiphase relation

Exercise (solution)

Coset decomposition of $Pm\bar{3}m$ in terms of $I4/mcm$ (**a**-**b**,**a**+**b**,2**c**)

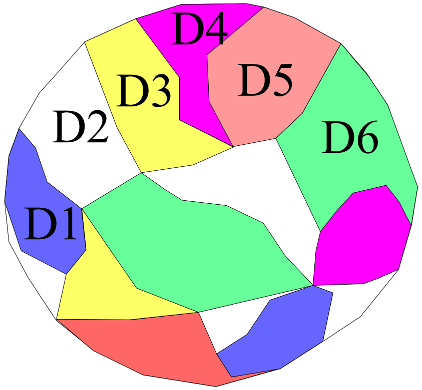


$$\begin{pmatrix}\mathbf{a}_1 & \mathbf{a}_2 & \mathbf{c}\end{pmatrix}\begin{pmatrix}1 & 1 & 0\\ \bar{1} & 1 & 0\\ 0 & 0 & 2\end{pmatrix}=\begin{pmatrix}\mathbf{a}'_1 & \mathbf{a}'_2 & \mathbf{c}'\end{pmatrix}$$

$Pm\bar{3}m = I4/mcm \cup 3^{+}{}_{[111]}I4/mcm \cup 3^{-}{}_{[111]}I4/mcm \cup \mathrm{t}(100)I4/mcm \cup \mathrm{t}(010)I4/mcm \cup \mathrm{t}(001)I4/mcm$

Exercise (solution)

$Pm\overline{3}m = I4/mcm \cup 3^{+}_{[111]}I4/mcm \cup 3^{-}_{[111]}I4/mcm \cup t(100)I4/mcm \cup t(010)I4/mcm \cup t(001)I4/mcm$



$D1 \rightarrow D2$: $3^{+}_{[111]}$

$D1 \rightarrow D3$: $3^{-}_{[111]}$

$D1 \rightarrow D4$: t(100)

$D1 \rightarrow D5$: t(010)

$D1 \rightarrow D6$: t(001)

$D2 \rightarrow D3$: $(D1 \rightarrow D2)^{-1} \rightarrow D3$: $3^{-}_{[111]} \cdot 3^{-}_{[111]} = 3^{+}_{[111]}$

$D2 \rightarrow D4$: $(D1 \rightarrow D2)^{-1} \rightarrow D4$: $t(100) \cdot 3^{-}_{[111]}$

$D4 \rightarrow D6$: $(D1 \rightarrow D4)^{-1} \rightarrow D6$: $t(001) \cdot t(\overline{1}00) = t(\overline{1}01)$

etc. etc. etc.

“Seeing” domains

Fourier transform of the content of the crystal

A crystal (periodic structure) is described as consisting of two functions (**r** is a vector spanning the direct space):

1. the real (direct) **periodic** lattice function $f_L(\mathbf{r})$, which is unity at each lattice node and zero elsewhere;
2. the **finite** electron density function $\rho(\mathbf{r})$, describing the content of a unit cell.

The crystal structure is the convolution of the periodic function $f_L(\mathbf{r})$ and the finite function $\rho(\mathbf{r})$

$$f_C(\mathbf{r}) = f_L(\mathbf{r}) * \rho(\mathbf{r})$$

The **Fourier transform** of the crystal structure gives the **diffraction pattern** produced when a radiation with suitable wavelength is sent onto the crystal. It is the product of the Fourier transforms of the lattice and of the unit cell content (**r*** is a vector spanning the reciprocal space)

$$F_C(\mathbf{r}^*) = T\,[f_L(\mathbf{r}) * \rho(\mathbf{r})] = T\,[f_L(\mathbf{r})] \cdot T\,[\rho(\mathbf{r})] = F_L(\mathbf{r}^*) \cdot F(\mathbf{r}^*)$$

$$F_L(\mathbf{r}^*) = T\left[f_L(\mathbf{r})\right] = \frac{1}{V} \sum_{h,k,l=-\infty}^{\infty} \delta\left(\mathbf{r}^* - \mathbf{r}^*_{hkl}\right) \quad F(\mathbf{r}^*) = T\left[\rho(\mathbf{r})\right] = \sum_{j=1}^{N} f_j(\mathbf{r}^*) \exp\left(2\pi i \mathbf{r}^* \cdot \mathbf{r}_j\right)$$

Fourier transform of the content of the crystal

$$F_C(\mathbf{r^*}) = F_L(\mathbf{r^*})\cdot F(\mathbf{r^*})$$

$$F_L\left(\mathbf{r}^*\right) = \frac{1}{V}\sum_{h,k,l=-\infty}^{\infty}\delta\left(\mathbf{r}^* - \mathbf{r}^*_{hkl}\right)$$

$$F\left(\mathbf{r}^*\right) = \sum_{j=1}^{N} f_j\left(\mathbf{r}^*\right)\exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{r}_j\right)$$

atomic nature

atomic positions

zero outside reciprocal lattice nodes

$$\int F\left(\mathbf{r}^*\right)\delta\left(\mathbf{r}^* - \mathbf{r}^*_{hkl}\right)dV_{\mathbf{r}^*} = F\left(\mathbf{r}^*_{hkl}\right) =$$

$$= \sum_{j=1}^{N} f_j\left(\mathbf{r}^*_{hkl}\right)\exp\left(2\pi i\mathbf{r}^*_{hkl}\cdot\mathbf{r}_j\right)$$

atomic nature

diffraction spot positions

atomic positions

The phase problem

$$\sum_{j=1}^{N} f_j(\mathbf{r}^*_{hkl})\exp\left(2\pi i\mathbf{r}^*_{hkl}\cdot\mathbf{r}_j\right) =$$

$$\sum_{j=1}^{N} f_j(hkl)\cos 2\pi\left(hkl\,|\,xyz\right) + i\sum_{j=1}^{N} f_j(hkl)\sin 2\pi\left(hkl\,|\,xyz\right) =$$

$$A(hkl) + iB(hkl) = \left|F(hkl)\right|\exp\left[i\varphi(hkl)\right]$$

Amplitude Phase

$$I(hkl) \propto \left|F(hkl)\right|^2$$

The information on the phase is not retrieved from a diffraction experiment!

Effect of translation on Fourier Transform

$\rho_T(\mathbf{r}) = \rho(\mathbf{r}\text{-}\mathbf{t})$ **t** = translation vector $F_T(\mathbf{r}^*) = \mathcal{T}[\rho_T(\mathbf{r})]$

$$F_T\left(\mathbf{r}^*\right) = \int \rho\left(\mathbf{r}-\mathbf{t}\right)\exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{r}\right)dV_{\mathbf{r}} =$$

$$= \exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{t}\right)\int \rho\left(\mathbf{r}-\mathbf{t}\right)\exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{r}-\mathbf{t}\right)dV_{\mathbf{r}} =$$

$$= F\left(\mathbf{r}^*\right)\exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{t}\right)$$

Translation of ρ(**r**) by a vector **t** in direct space is equivalent to modifying the Fourier transform by the **phase** factor exp(2πi**r***·**t**) in reciprocal space, without change in the modulus |F(**r***)|, but the real and imaginary part of F(**r***) are multiplied by cos(2π**r***·**t**) and sin(2π**r***·**t**) respectively. A description of a transform is thus *origin dependent*.

How can we see domain states?

$$F_T\left(\mathbf{r}^*\right) = F\left(\mathbf{r}^*\right)\exp\left(2\pi i\mathbf{r}^*\cdot\mathbf{t}\right)$$

$$I(hkl) \propto |F(hkl)|^2$$

G group of the parent phase

$\downarrow$

H group of the daughter phase

translationengleiche subgroup
(same lattice, lower point group)

Twin domains
(differing by orientation)

Visible in the diffraction pattern, which shows the overlap of two (or more) lattices differently oriented.

klassengleiche subgroup
(sublattice, same point group)

Antiphase domains
(differing by position)

Invisible in the diffraction pattern
(effect on the ***phase***)
Visible by electron microscopy

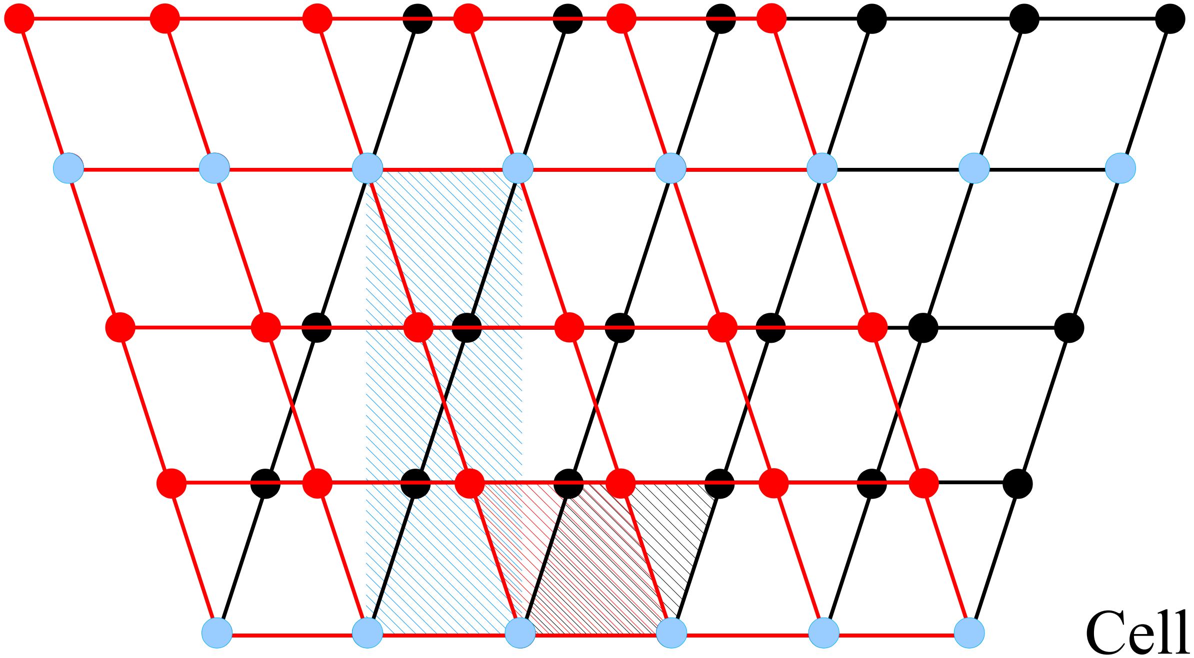
Twinning

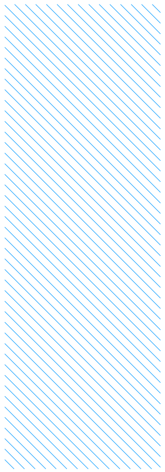
Probability occurrence of twins in term of the reticular theory

- 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 reticular theory allows a general approach in terms of lattice restoration as a necessary (not sufficient) condition.
- We need parameters to evaluate the degree of lattice restoration: these are the twin index and the obliquity.

Twin lattice

The twin lattice is the sublattice common to the twinned domain states based on the twin element (plane, axis) and the (quasi)-perpendicular lattice element (direction, plane).

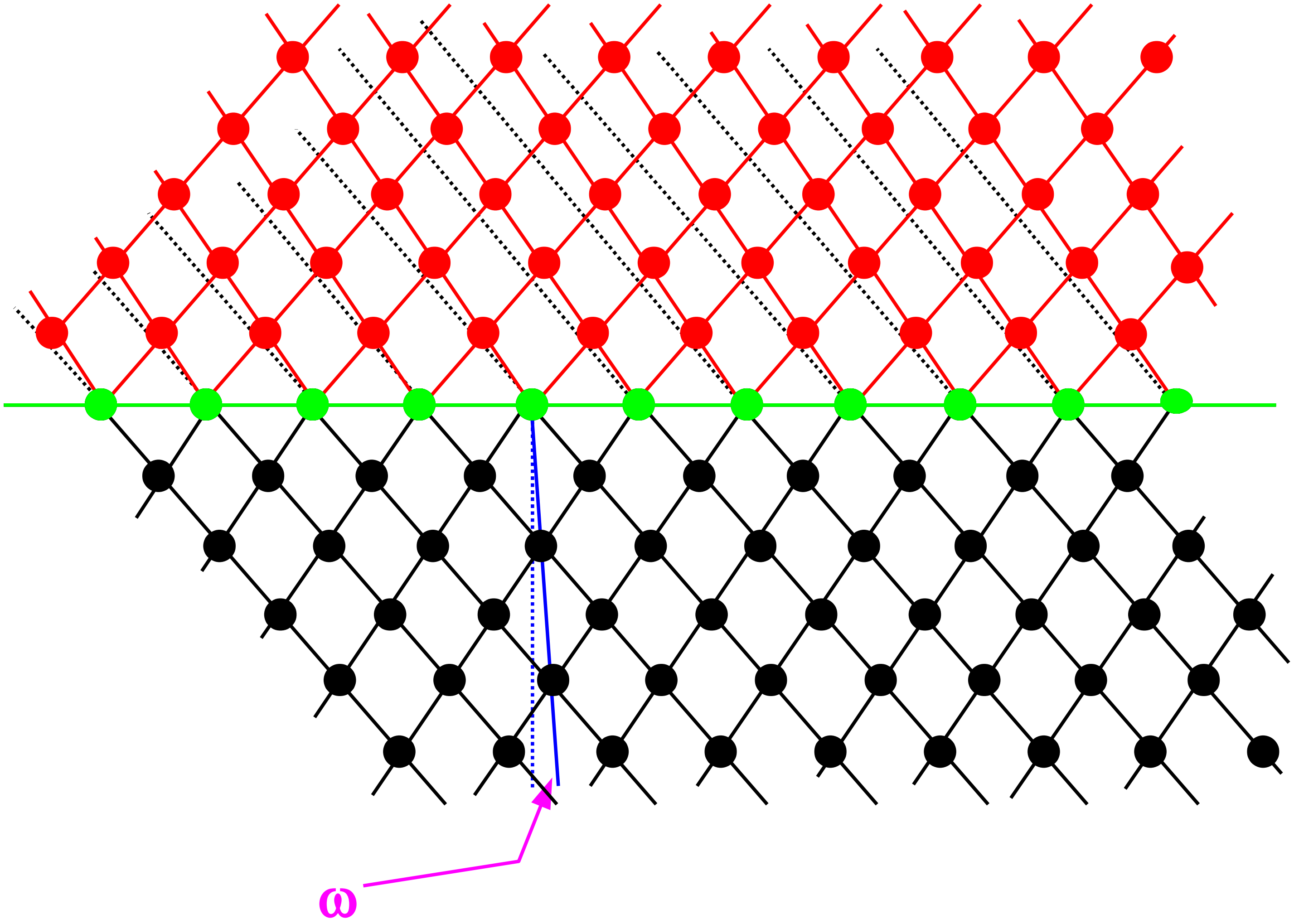




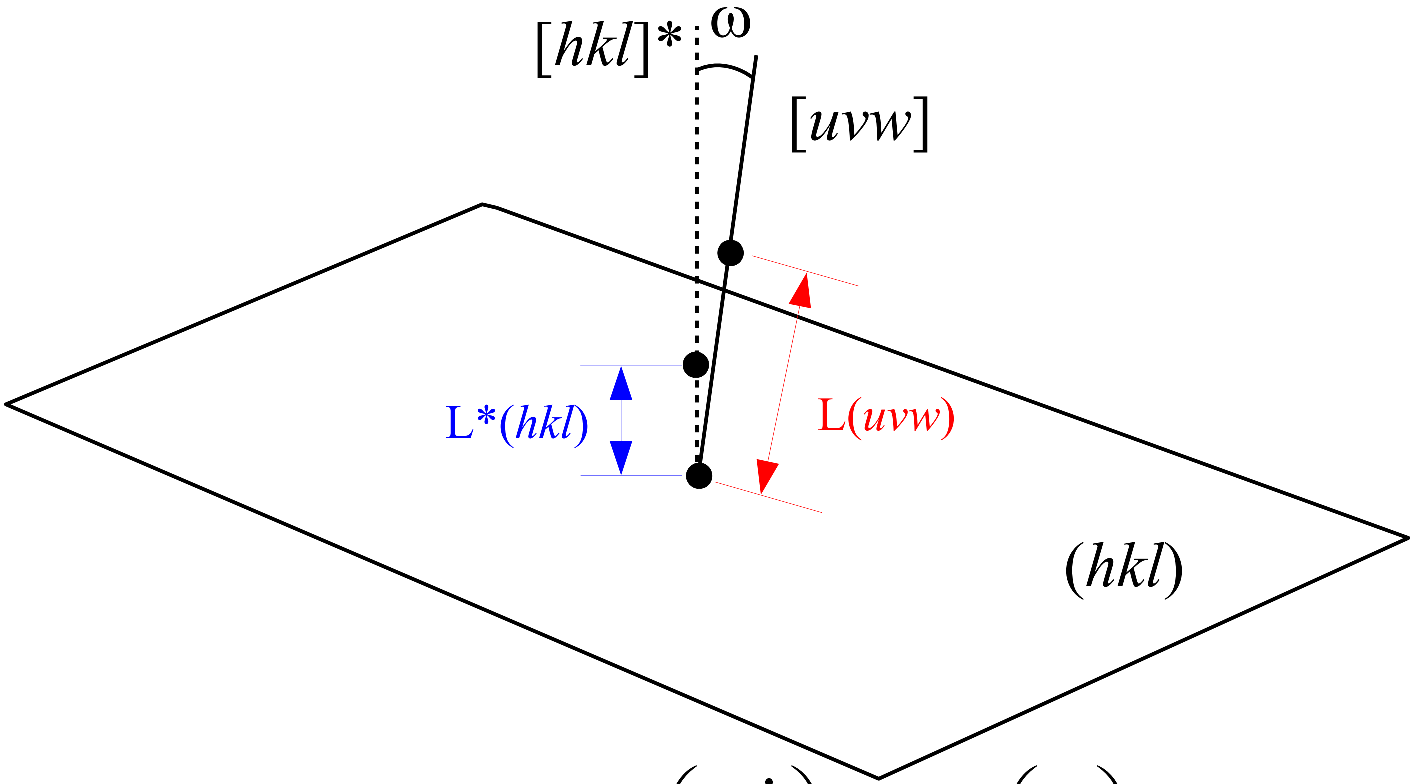
Cell of the twin lattice

One node out of *n* restored by the twin operation: we say that **the twin index is *n*** (3 in this example)

Definition of obliquity



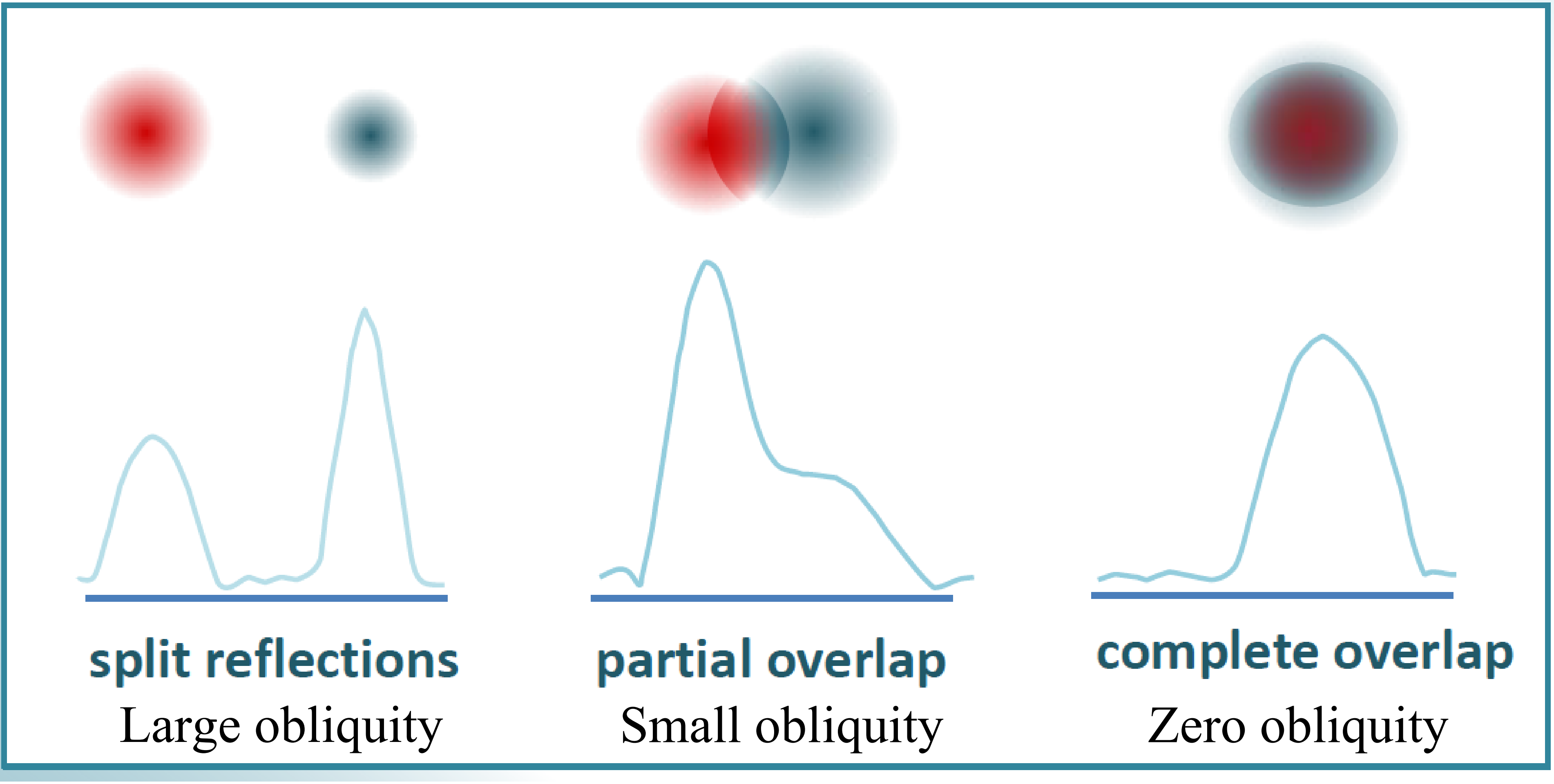
Computation of the obliquity



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

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

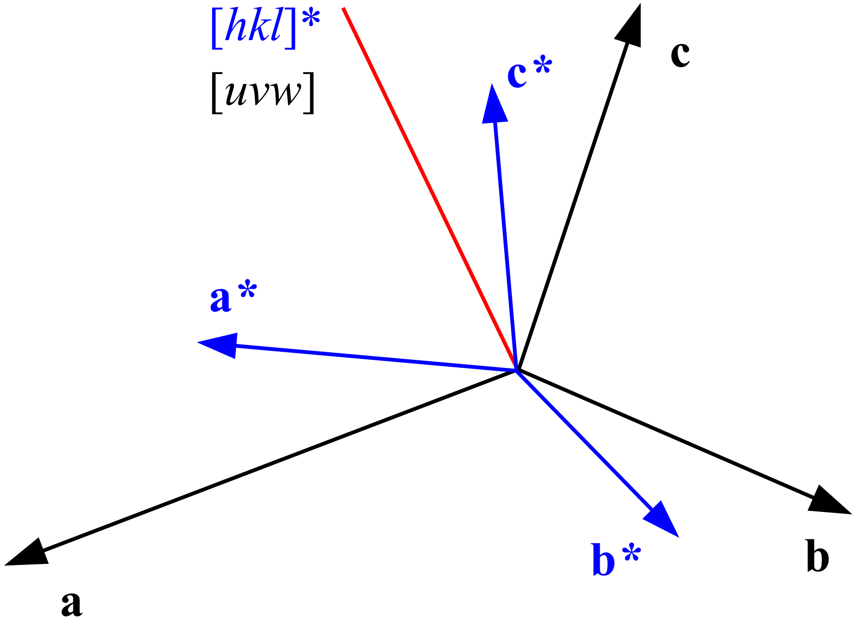
Effect of the obliquity on the diffraction pattern



Source: Andrea Thorn, Computing School 2011

How to find the direction [*uvw*] quasi-perpendicular to (*hkl*) necessary to compute the obliquity?

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



How?

Easy!

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

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

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

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

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

Easy!

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

$$\left(hkl\right)\mathbf{G}^{*}\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}3=\left(uvw\right)\begin{pmatrix}\boldsymbol{a}\\ \boldsymbol{b}\\ \boldsymbol{c}\end{pmatrix}$$

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

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

Basis transformation (general)

$$\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\mathbf{P} = \begin{pmatrix}\mathbf{a'} & \mathbf{b'} & \mathbf{c'}\end{pmatrix}$$

$$\mathbf{G}' = \begin{pmatrix}\mathbf{a'}\\ \mathbf{b'}\\ \mathbf{c'}\end{pmatrix}\begin{pmatrix}\mathbf{a'} & \mathbf{b'} & \mathbf{c'}\end{pmatrix} = \mathbf{P}^t\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{pmatrix}\begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\mathbf{P} = \mathbf{P}^t\mathbf{G}\mathbf{P}$$

$$\mathbf{P} = \begin{array}{cc} & \begin{array}{ccc}\mathbf{a}' & \mathbf{b}' & \mathbf{c}'\end{array} \\ \begin{array}{c}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{array} & \begin{bmatrix} a'_a & b'_a & c'_a \\ a'_b & b'_b & c'_b \\ a'_c & b'_c & c'_c \end{bmatrix}\end{array}$$

Check the determinant!

Basis transformation (twinning)

$$\mathbf{P} = \begin{bmatrix} u_{\perp} & u_1 & u_2 \\ v_{\perp} & v_1 & v_2 \\ w_{\perp} & w_1 & w_2 \end{bmatrix}$$

Direction quasi-perpendicular to (*hkl*)

Directions in the (*hkl*) plane

$hx + ky + lz = 0$: (*hkl*) plane passing through the origin

[*uvw*]: direction passing through nodes 000, *uvw*, 2*u*2*v*2*w*….

$hu + kv + lw = 0$: condition for the [*uvw*] direction to be contained in the (*hkl*) plane

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!

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

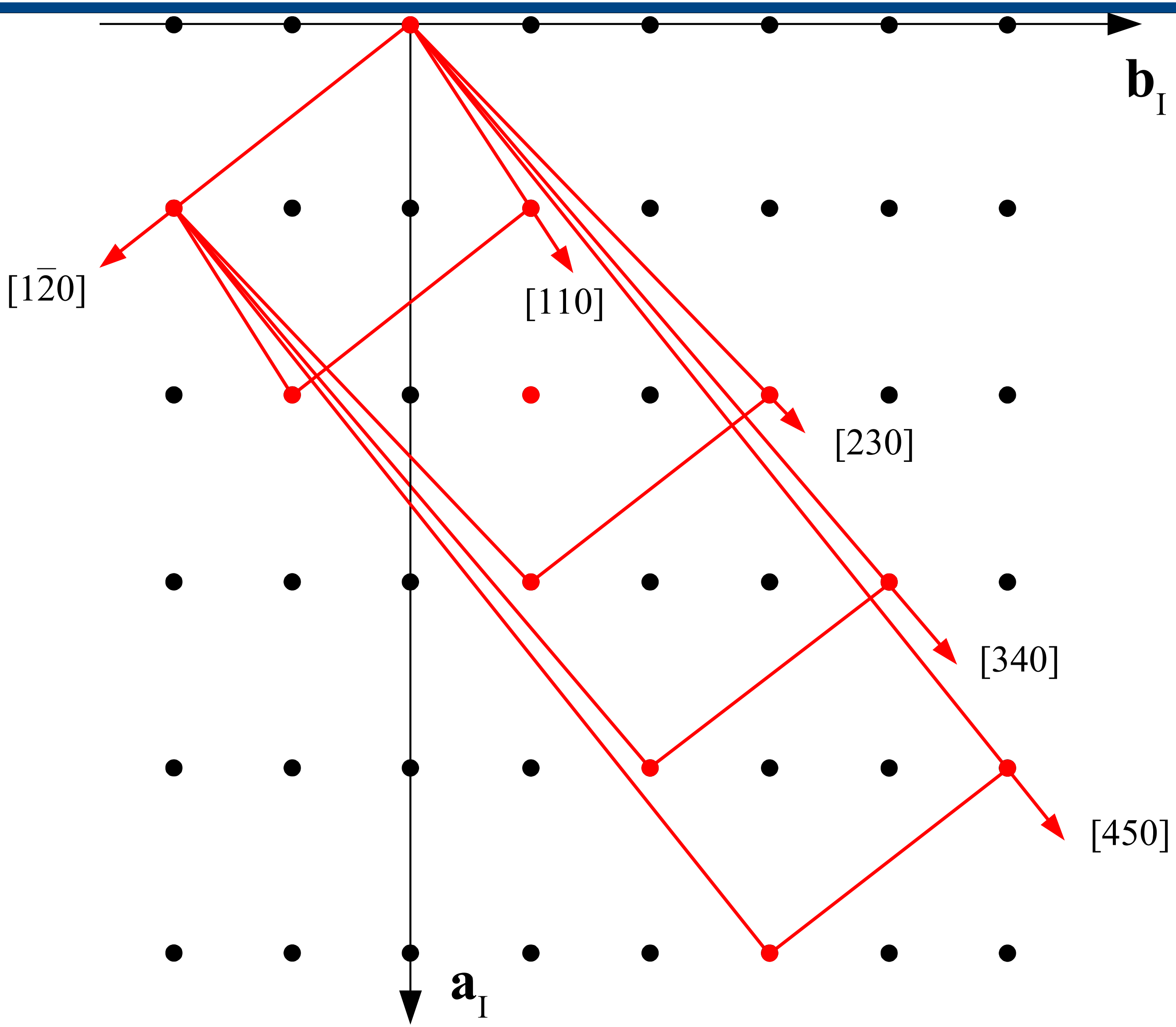
u	***v***	***v/u***
1	1	1
1	2	2
2	3	1.5
3	4	1.333
4	5	1.25

Calculate the obliquity

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

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

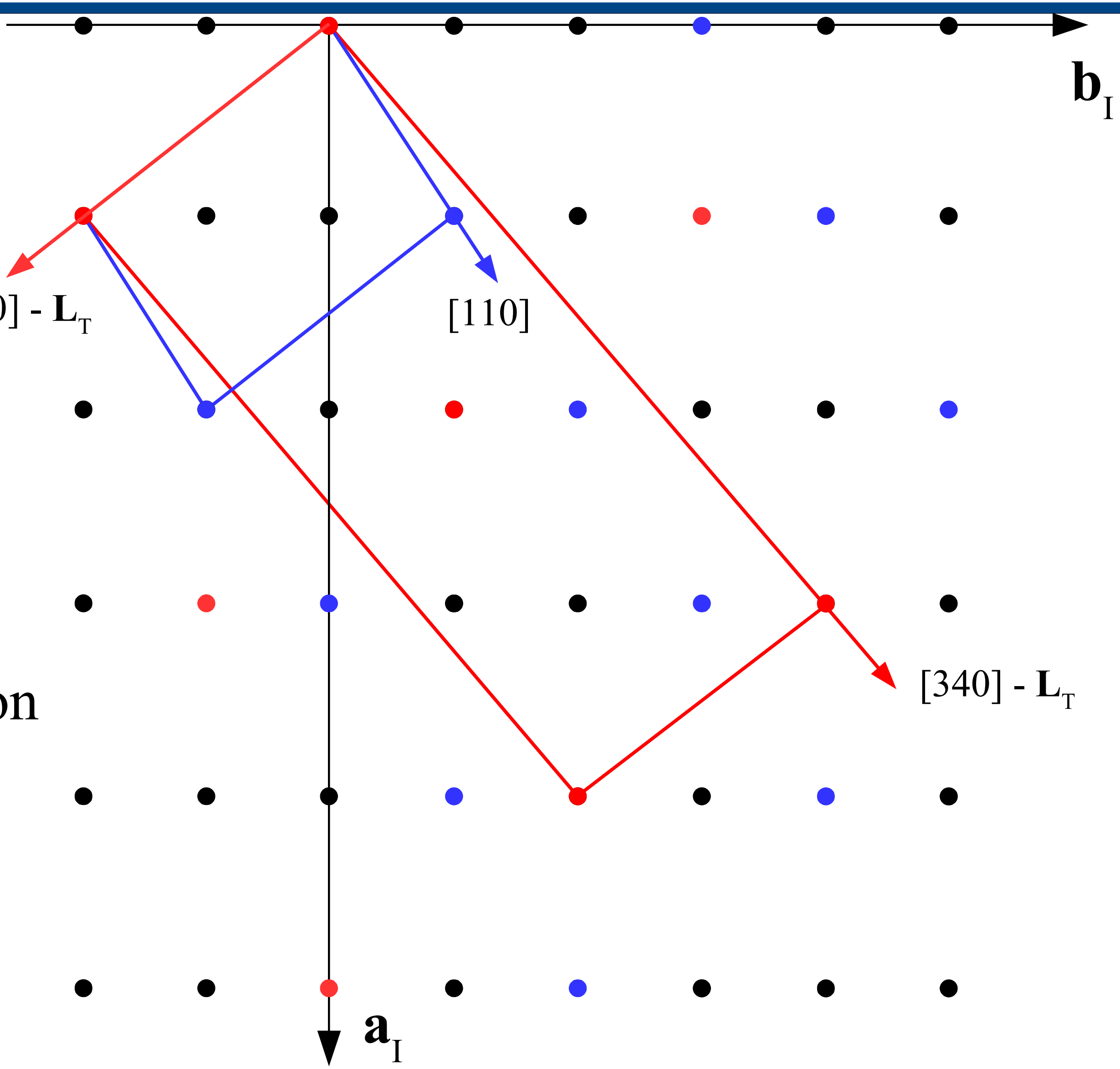
uvw	ω	***n***
110	5.36°	3
~~230~~	~~5.86°~~	~~7~~
340	2.50°	5
~~450~~	~~0.69°~~	~~13~~

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....

$$\begin{pmatrix} \boldsymbol{a} & \boldsymbol{b} & \boldsymbol{c} \end{pmatrix} \mathbf{P} = \begin{pmatrix} \boldsymbol{a}' & \boldsymbol{b}' & \boldsymbol{c}' \end{pmatrix}$$

$$\mathbf{G}' = \begin{pmatrix} \boldsymbol{a}' \\ \boldsymbol{b}' \\ \boldsymbol{c}' \end{pmatrix} \begin{pmatrix} \boldsymbol{a}' & \boldsymbol{b}' & \boldsymbol{c}' \end{pmatrix} = \mathbf{P}^t \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{pmatrix} \begin{pmatrix} \boldsymbol{a} & \boldsymbol{b} & \boldsymbol{c} \end{pmatrix} \mathbf{P} = \mathbf{P}^t\mathbf{G}\mathbf{P}$$

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

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

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

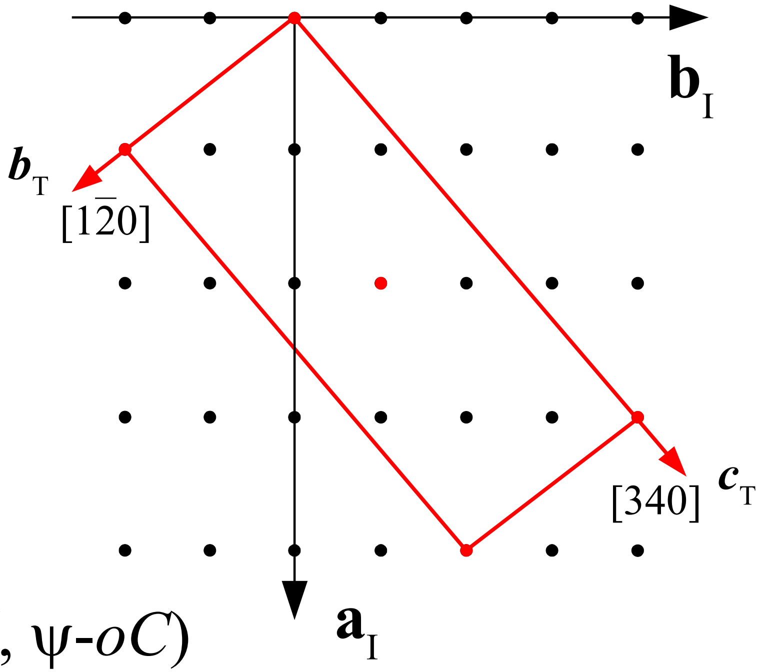
$$= \begin{vmatrix} 0 & 0 & c^2 \\ a^2 & -2b^2 & 0 \\ 3a^2 & 4b^2 & 0 \end{vmatrix} \begin{vmatrix} 0 & 1 & 3 \\ 0 & \bar{2} & 4 \\ 1 & 0 & 0 \end{vmatrix} = \begin{vmatrix} c^2 & 0 & 0 \\ 0 & a^2+4b^2 & 3a^2-8b^2 \\ 0 & 3a^2-8b^2 & 9a^2+16b^2 \end{vmatrix}$$

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

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

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

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....

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

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-obliqui/ty TLQS twinning

b ≈ c