Pseudo translation and Twinning

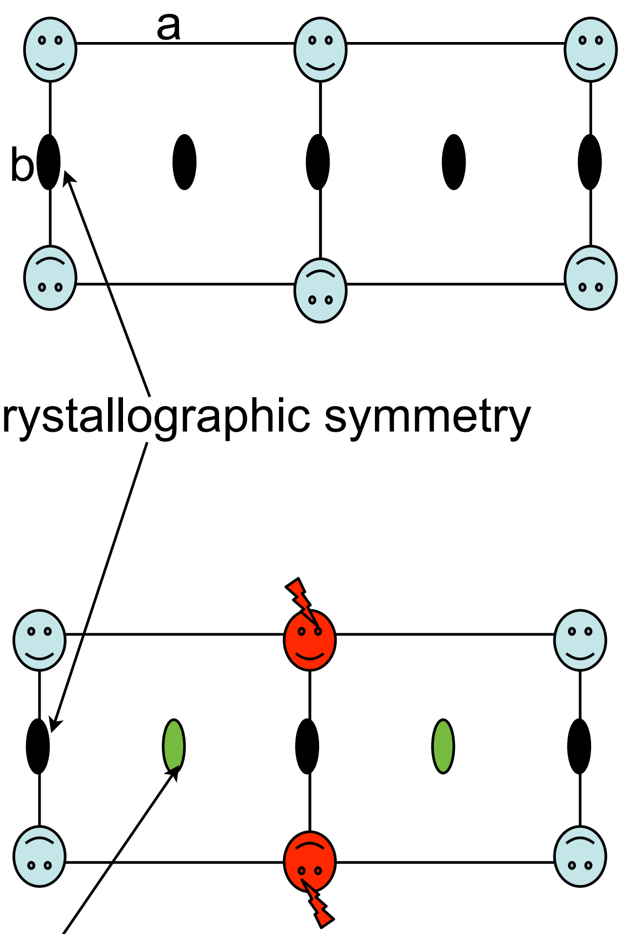
Crystal peculiarities

- Pseudo translation
- Twin
- Order-disorder

Pseudo Translation

Pseudo translation

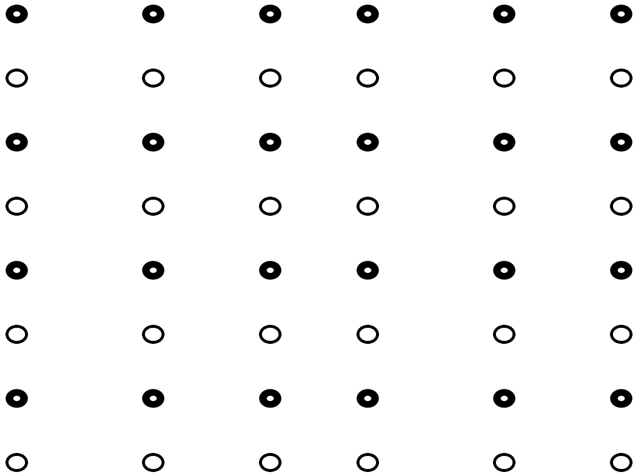
Real space



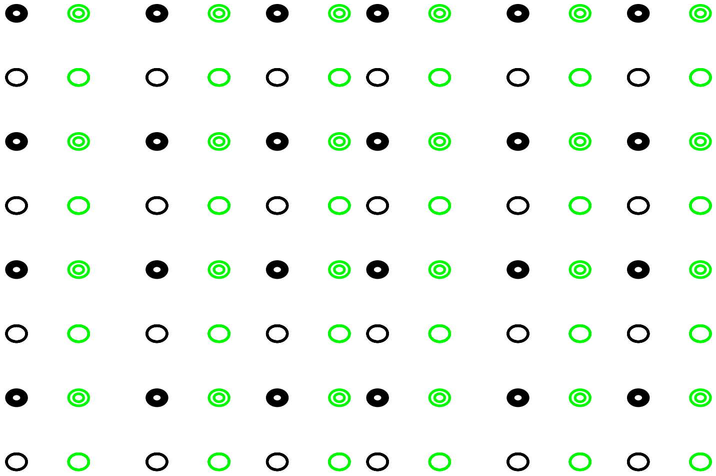
Crystallographic symmetry

Non-crystallographic symmetry

Reciprocal space



Distance between spots: 1/a, 1/b

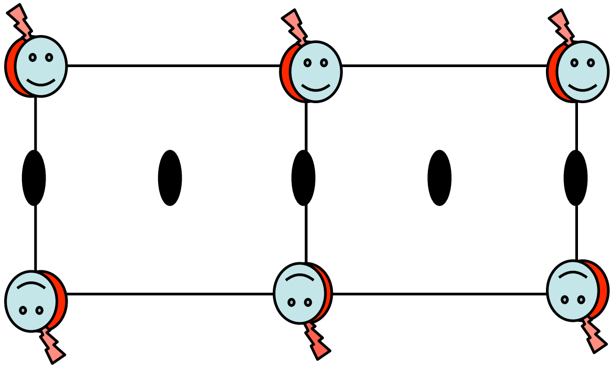


Distance between spots: 1/(2a), 1/b

Every second reflection is weak.

Why PST may cause problem?

If weak reflections are ignored then crystal lattice will be twice smaller and resultant electron density (and atomic model) will be average of two slightly different molecules

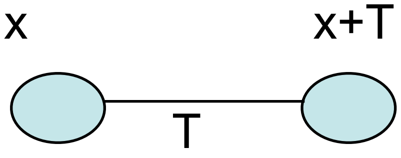


Sometimes it may be useful to index in smaller cell, solve molecular replacement problem and then go back to larger cell.

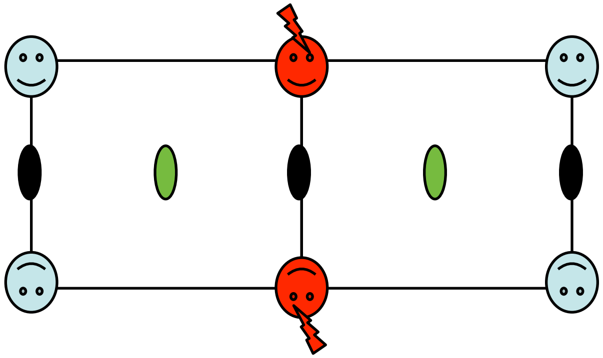
Why PST may cause problem?

Most statistics in crystallography relies on simple assumptions: 1) Crystal contains atoms; 2) Atoms are uniformly and randomly distributed over whole unit cell. When there is a pseudo translation then for every atom at a position x there is another atom at the position x+T. Thus assumption 2) breaks down. It changes statistical properties of intensities.

As a result many tests (e.g. twinning) based on these assumptions may give misleading results.



Why PST may cause problem?

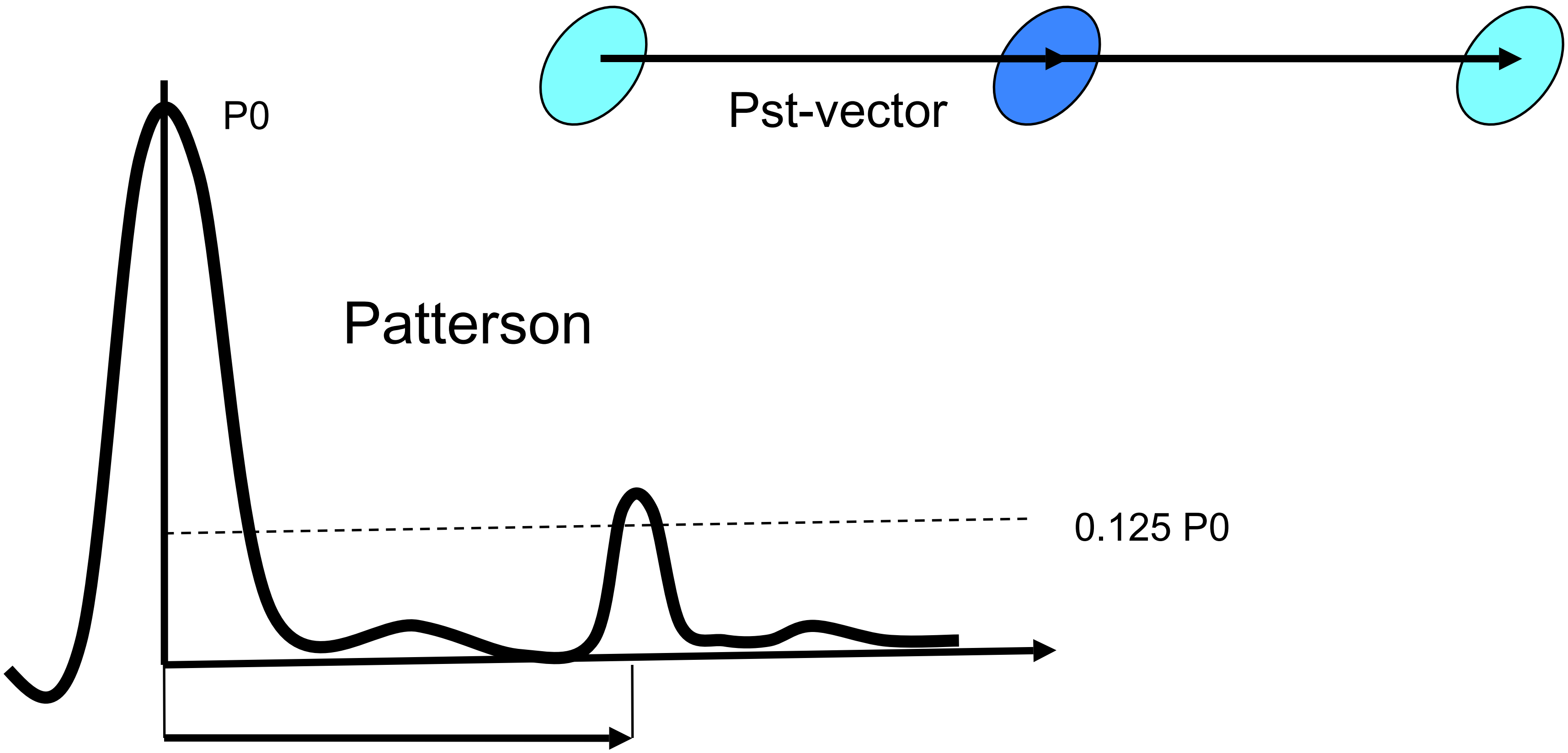


Molecular replacement programs may confuse crystallographic and non-crystallographic symmetry. It may result in false origin solutions.

If such problem occurs then refinement may stuck at high R-factors. In these cases program *zanuda* written by Andrey Lebedev may help. It is available on YSBL online software site:

http://www.ysbl.york.ac.uk/YSBLPrograms/index.jsp

PST and Patterson



Cell

Pst-vector

P0

Patterson

0.125 P0

Pst-vector

Why PST may cause problem?

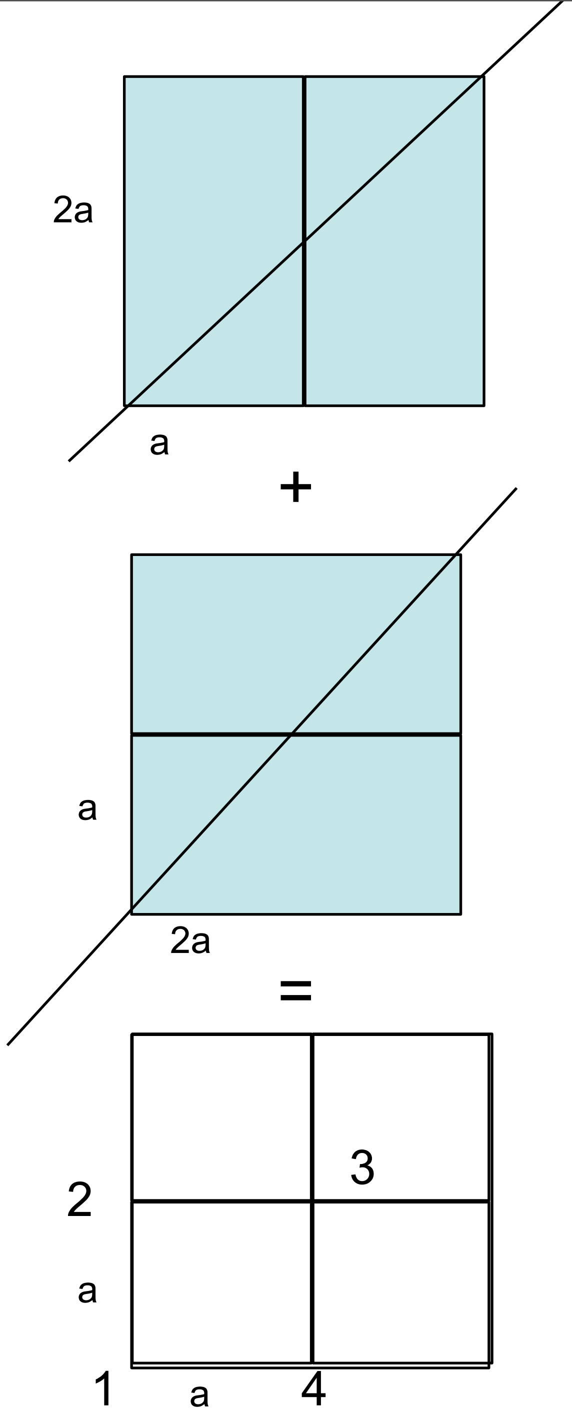
Pseudo translation (PST) may cause problems in molecular replacement. Moreover in the presence of PST the solution may be in the wrong origin. Refinement usually does not have much problem once initial structure have been found (or built).

Note that there may be other sources of apparent pseudotranslation:

1) Non-merohedral twin
2) Helices, DNA
3) Order-disorder

If accidentally one of the cell edges - b is twice larger than the cell edge a and contents of the crystal allows then we may have two orientation of the crystal. In this case it may happen that indexing gives cell dimensions (2a,2a). Point 1 and 4 are related by translation in the first crystal; point 1 and 2 are related in the second crystal and point 4 and 3 are related in neither crystals.

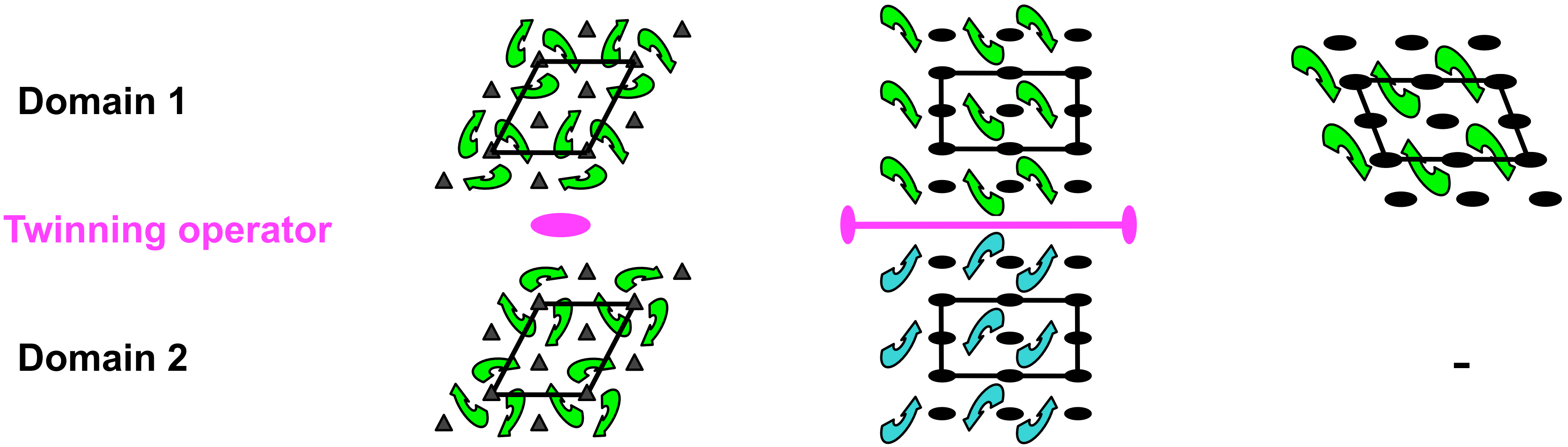
Another misindexing option is (a,a). In this case the cell will not be big enough to accommodate the molecule.



Twinning

merohedral and pseudo-merohedral twinning

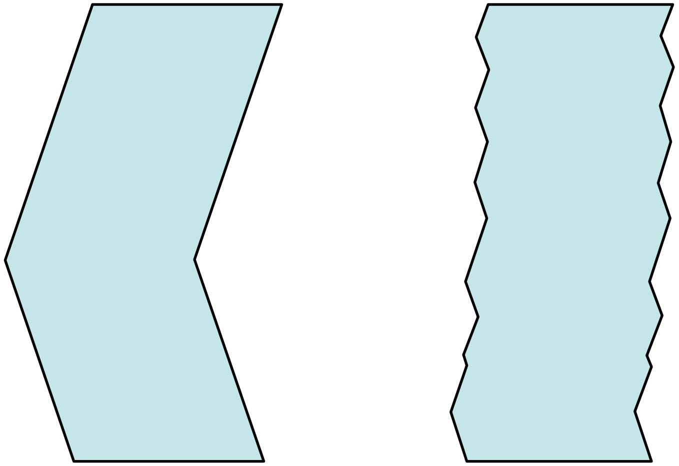
Crystal symmetry:	P3	P2	P2
Constrain:	-	β = 90º	-
Lattice symmetry *: (rotations only)	P622	P222	P2
Possible twinning:	merohedral	pseudo-merohedral	-



Crystal lattice is invariant with respect to twinning operator.

The crystal is NOT invariant with respect to twinning operator.

The whole crystal: twin or polysynthetic twin?



	twin	polysynthetic twin
A single crystal can be cut out of the twin:	yes	no

The shape of the crystal suggested that we dealt with polysynthetic OD-twin

Twinning

If we have only two domains related with twin operator then observed intensities will be

$$I_{T1} = (1-\alpha)I_1 + \alpha I_2$$
$$I_{T2} = (1-\alpha)I_2 + \alpha I_1$$

I_{T1} and I_{T2} are observed intensities, I_1 and I_2 are intensities from single crystals, α is proportion of the second domain. α is between 0 and 0.5. When it is 0.5 then twin called perfect twin.

In principle these equations can be solved and I_1 and I_2 (intensities for single crystal) can be calculated. It is called detwinning. It turns out that detwinning increases errors in intensities. Also, completeness after detwinning can decrease substantially. Moreover when $\alpha=0.5$ it is impossible to detwin.

For some purposes (e.g. for phasing, sometimes for molecular replacement) detwinning may give reasonable results. For refinement general rule is to avoid detwinning and use the data directly. Almost all known refinement programs can handle twinning to a certain degree.

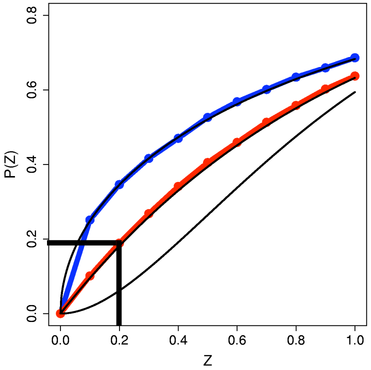
Effect on intensity statistics

Take a simple case. We have two intensities weak and strong. When we sum them then we we will have four options w+w, w+s, s+w, s+s. So we will have one weak, two medium and one strong reflection.

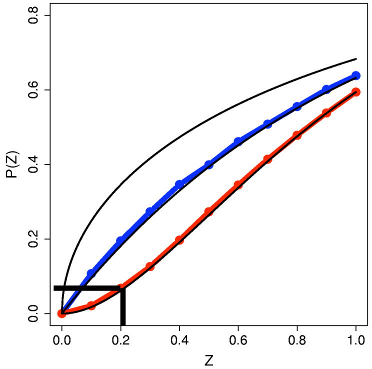
As a results of twinning, proportion of weak and strong reflections becomes less and the number of medium reflections increases. It has effect on intensity statistics

Example of effect of twinning on cumulative distributions

Cumulative distribution is the proportion (more precisely probability) of data below given values - F(x) = P(X<x).



No twinning. Around 20% of acentric reflections are less than 0.2.



Perfect twinning. Only around 5% of acentric reflections are less than 0.2.

Cumulative distribution of normalised structure factors
Red lines - of acentric reflections,
Blue lines - centric reflections

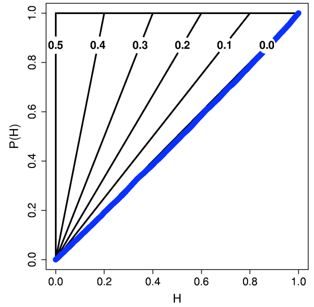
H-test

T.Yeat’s is very popular and useful test. It is based on cumulative distribution of

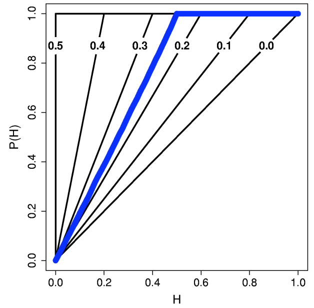
$$H = |I_{T1}-I_{T2}|/(I_{T1}+I_{T2})$$

When there is no twinning then cumulative distribution of H is represents a diagonal line (I.e. H is distributed uniformly between 0 and 1.

SFCHECK uses this test but it produces inverted picture.



No twinning

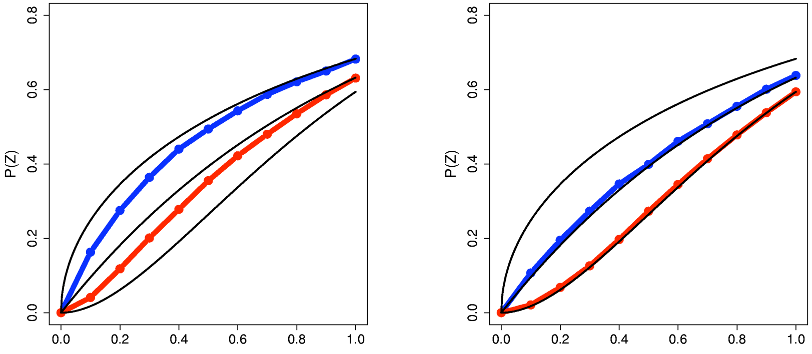


Partial twinning

Twinning and Pseudo Rotation

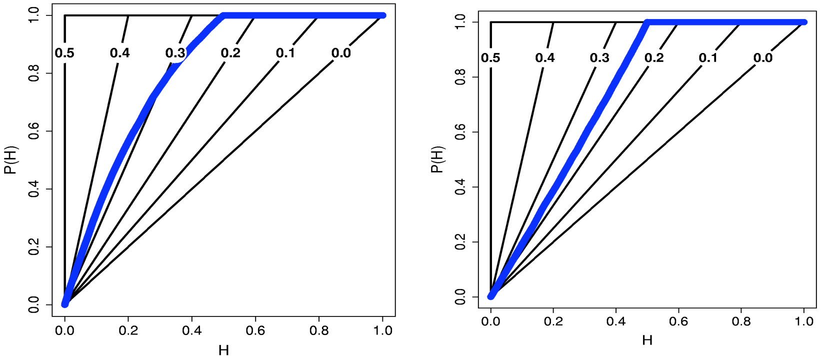
In many cases twin symmetry is (almost) parallel to non-crystallographic symmetry. In these case we need to consider the effects of two phenomena: twinning and NCS.
Because of NCS two related intensities (I_1 and I_2) will be similar (not identical) to each other and because of twinning proportion of weak intensities will be smaller. It has effect on cumulative intensity distributions as well as on H-test

Perfect twinning



Cumulative intensity distribution with and without interfering NCS

Partial twinning



H-test with and without interfering NCS

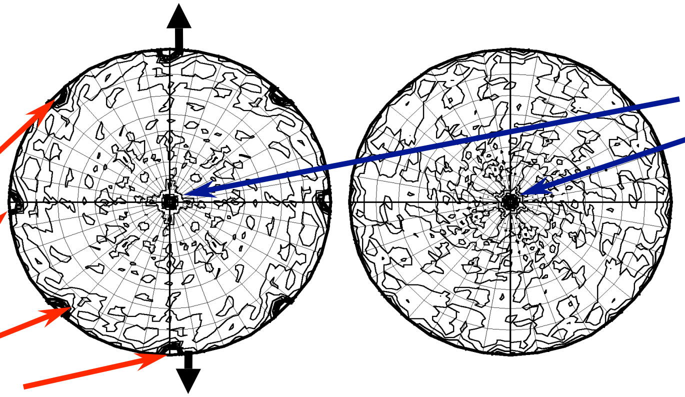
Twins: Self-Rotation Function

Figures show sections of the self-rotation function corresponding to two-fold axes

Experimental data

Model (single domain)

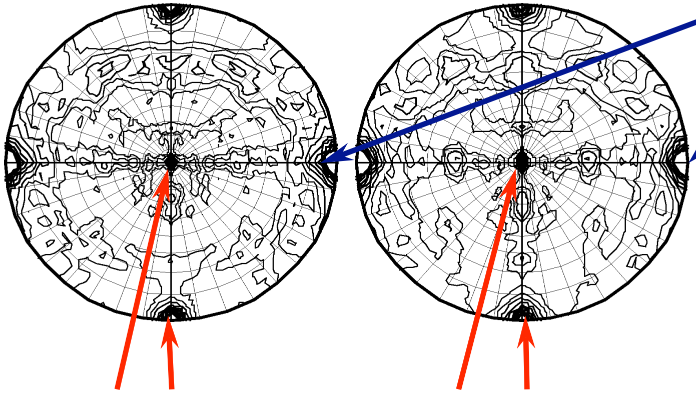
- PDB code 1l2h
- Spacegroup $P4_3$
- 1 molecule per AU
- Merohedral twinning



Crystallographic two-fold axis

Four equivalent twinning two-fold axes

- PDB code 1igj
- Spacegroup $P2_1$
- NCS (**Pseudosymmetry**): 2 monomers per AU
- Pseudo-merohedral twinning

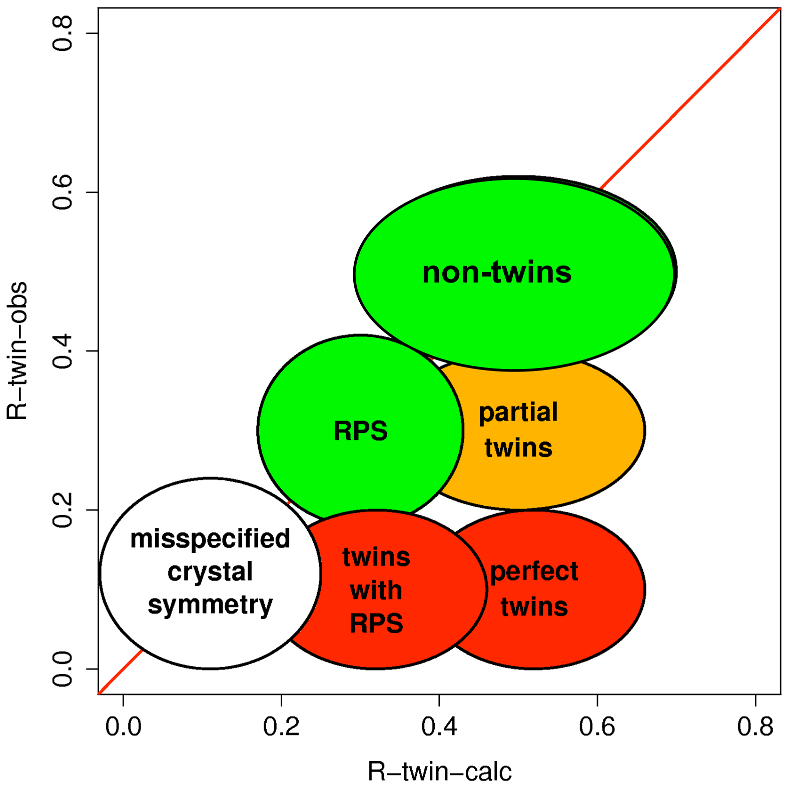


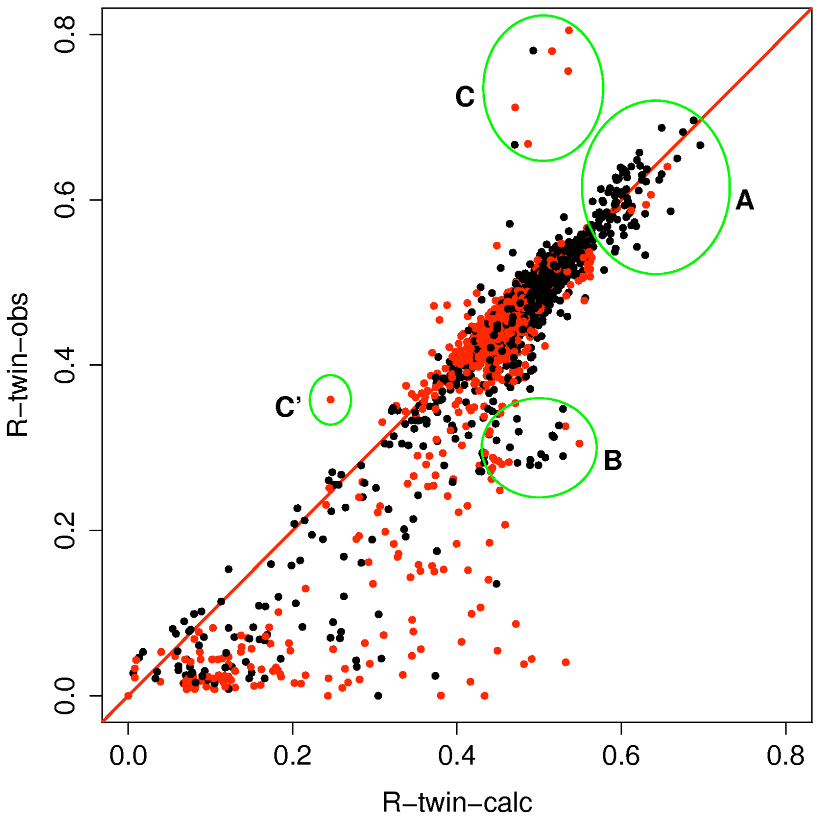
Crystallographic two-fold axis

Pseudosymmetry and twinning

Pseudosymmetry

RvR-plot





$$R_{twin} = \frac{\sum_h |I(h) - I(S_{twin}h)|}{2\sum_h I(h)}$$

$$R_{twin}^{obs} :: I \rightarrow I^{obs}$$

$$R_{twin}^{calc} :: I \rightarrow I^{calc}$$

A: translational NCS
B: mislabeling F→I
C,C': mislabeling I→F

Red: (potential) merohedral twins
Black: (potential) pseudomerohedral twins

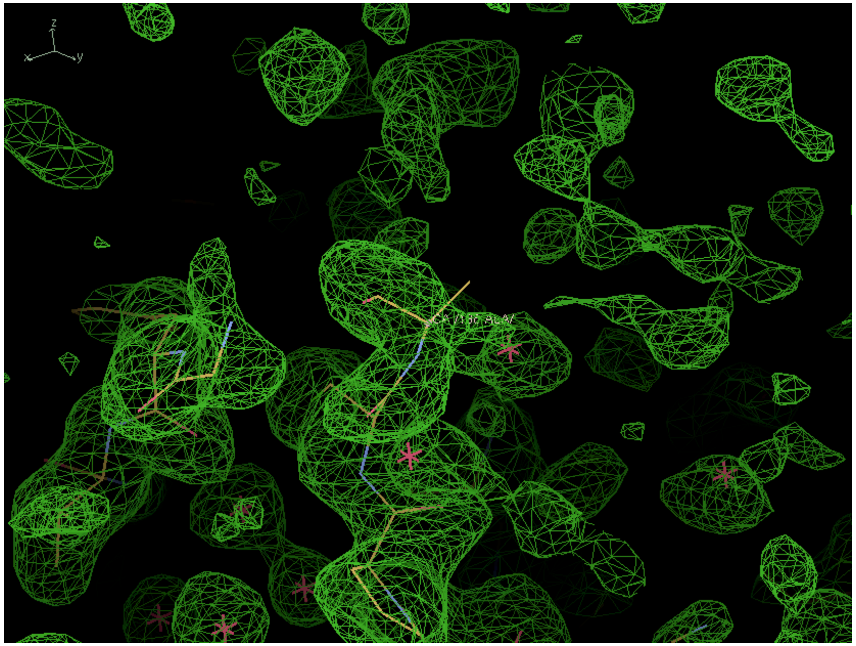
Effect of twinning on electron density

Using twinning in refinement programs is straightforward. It improves statistics substantially (sometimes R-factors can go down by 10%. However improvement of electron density is not very dramatic. It may improve electron density in weak parts but in general do not expect too much. Especially when twinning and NCS are close then improvements are marginal.

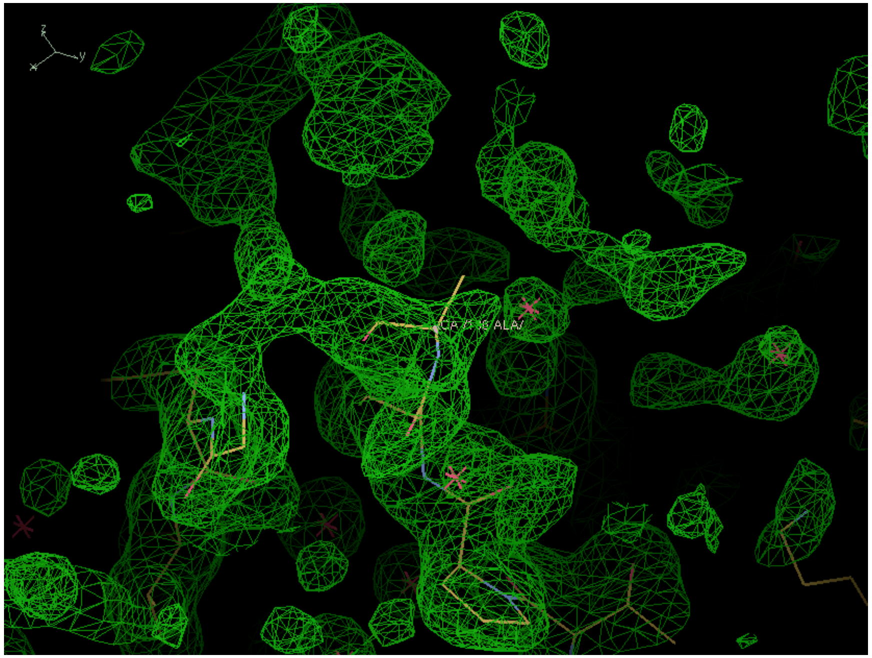
Electron density: 1rxf

We will see occasionally this

“refmac” map

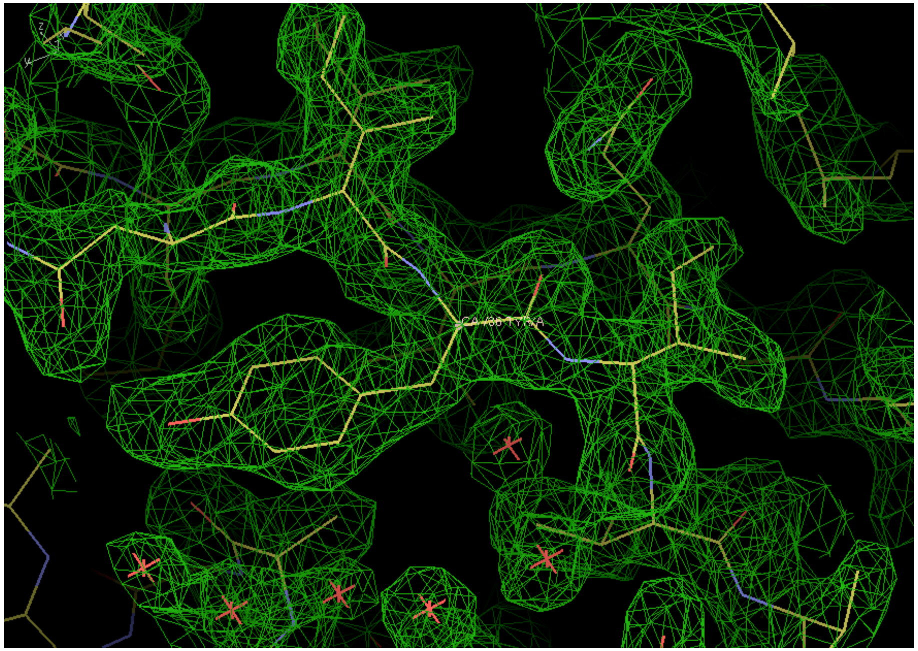


“twin” map

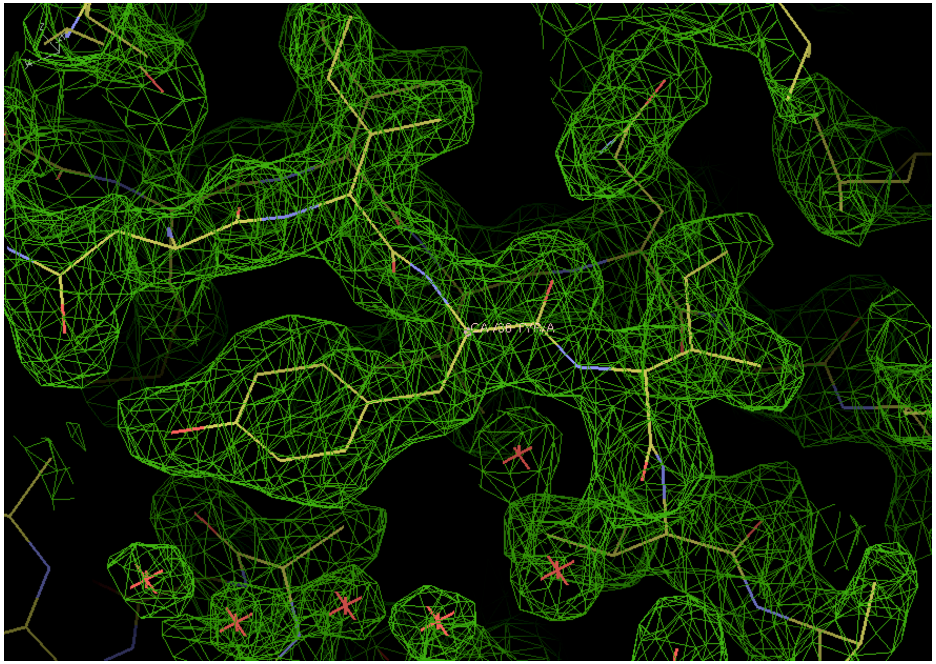


Electron density: 1jrg
More usual and boring case

"refmac" map



"twin" map



Effect of twin on electron density: Noise level. Very, very approximate

$$|F_t|e^{i\phi} \approx |F_R|e^{i\phi} + \alpha(|F_w| - |F_R|)e^{i\phi}$$

F_t - twinned structure factor
F_R - structure factor from “correct” crystal
F_W - structure factor from “wrong” crystal

The first term is correct electron density the second term corresponds to noise.
When twin and NCS are parallel then the second term is even smaller.