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Lecture course on crystallography, 2015

Lecture 8: Introduction to space symmetry operations and space groups

REMINDER: Types of symmetry operation

According to the type of movement there are different types of symmetry operations

1. Point symmetry: AT LEAST one point is fixed during the movement of the object

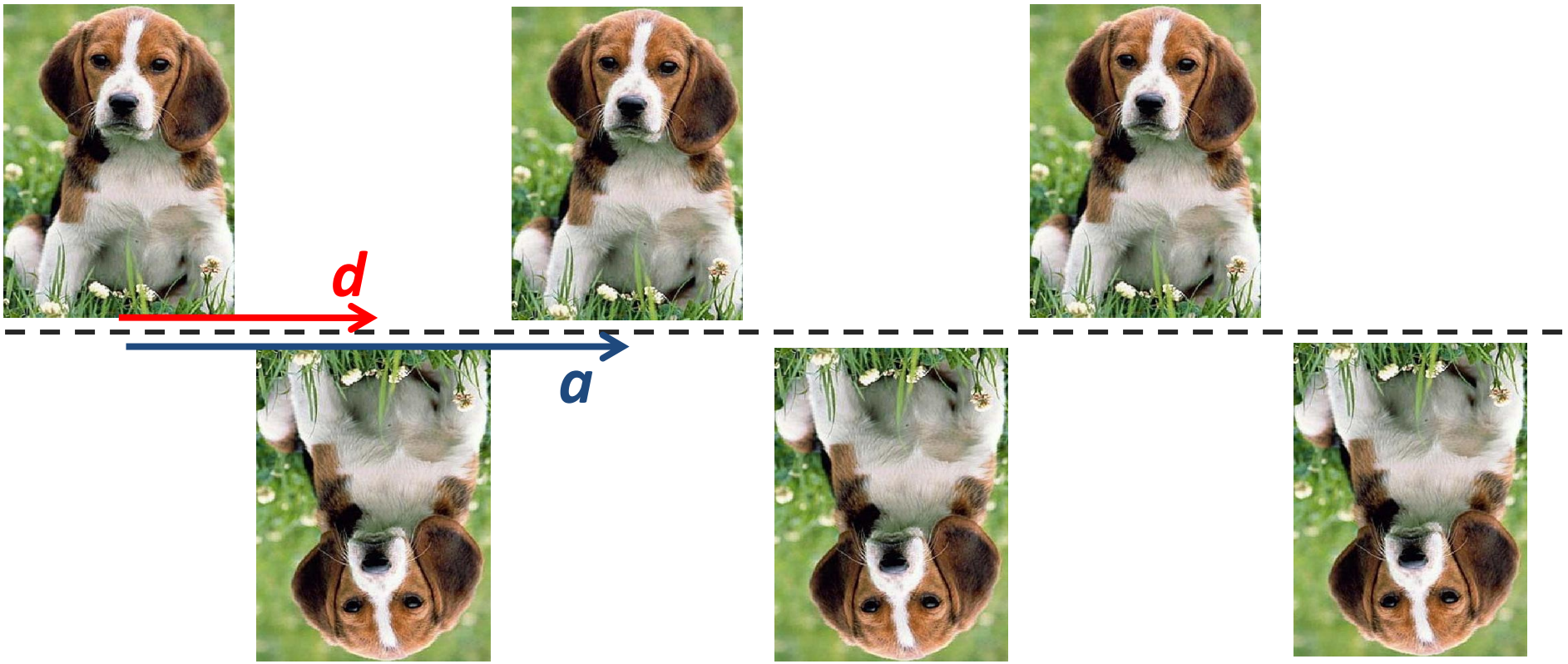
- *Rotation*
- *Reflection*
- *Inversion*
- *Combination of any above*

2. Space symmetry: no points are fixed during the movement of the object

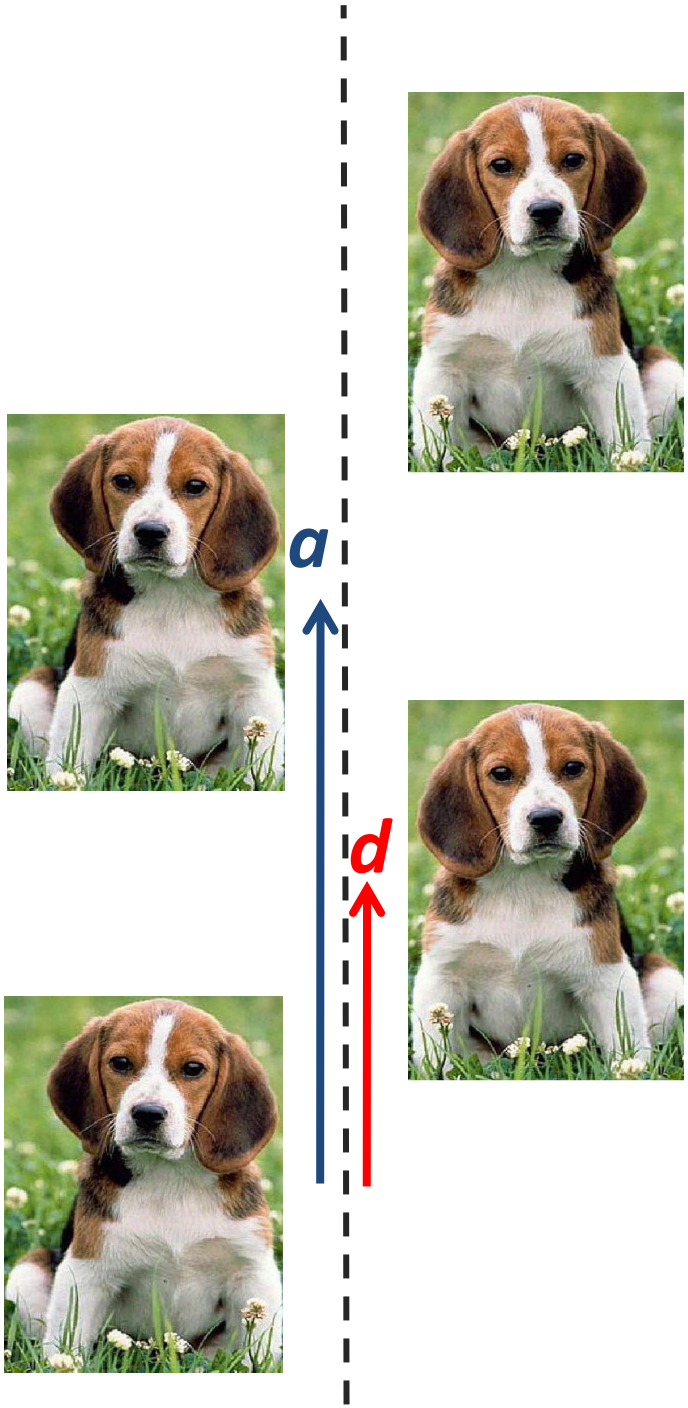
- *Translation (lattice translation)*
- *Combination of translation and any kind of point symmetry operations*

Space symmetry operations: glide planes

Glide plane is the symmetry element associated with the combination of a mirror and translation along the mirror.



d is the displacement, a=2d is a periodicity of a system



The displacement within a glide plane is always half the periodicity of the system in the direction of the displacement

Notations for the glide plane

Notation	Graphical symbol	Actual meaning
a, b, c		The glide is along basis vectors ***a***, ***b*** or ***c***
g		The glide is along the line (in 2D)
n		The glide is along one of the diagonal [110]
d		The glide is along the diagonal [111]

Reading symmetry diagrams containing glide planes

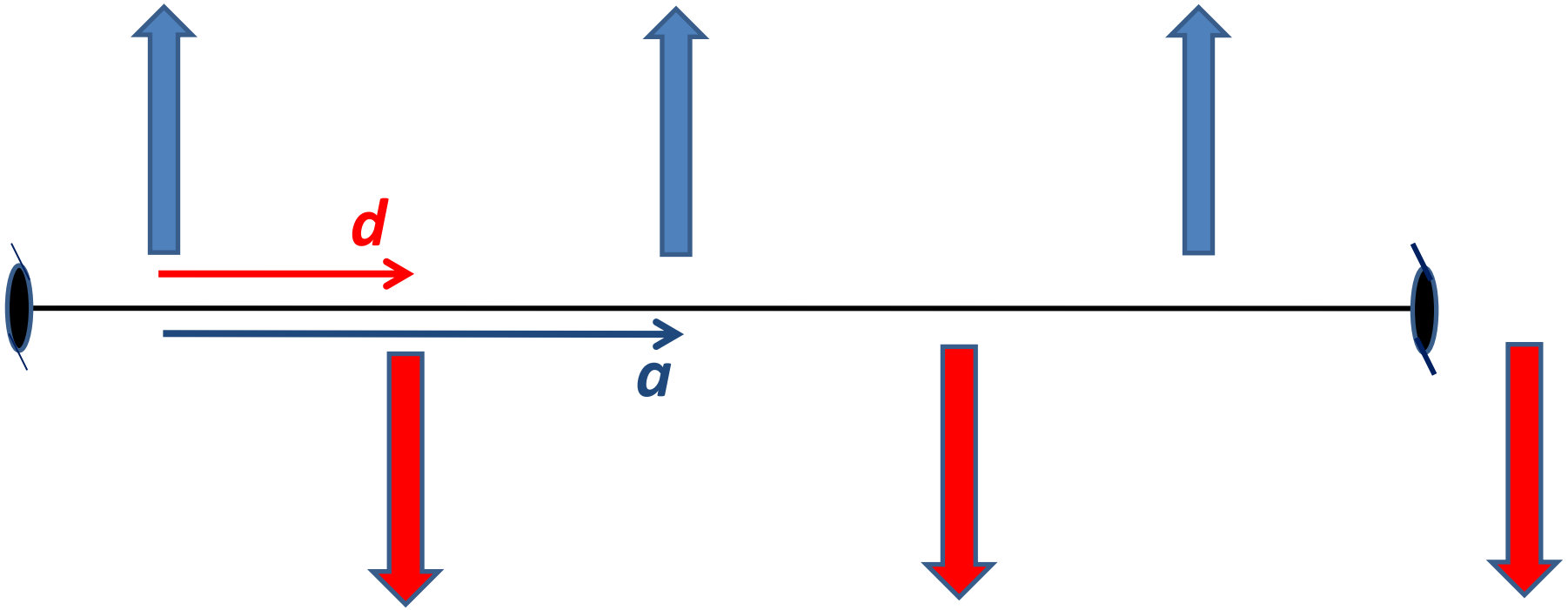
1. Glide direction is parallel to the line (for *a b* or *c* planes)

2. Glide direction is perpendicular to the projection plane (for *a b* or *c* planes)

3. Glide direction between the directions 1 and 2 (for *n* planes)

Screw axis

Screw axis is the symmetry element associated with the combination of a rotation axis and translation along the axis.

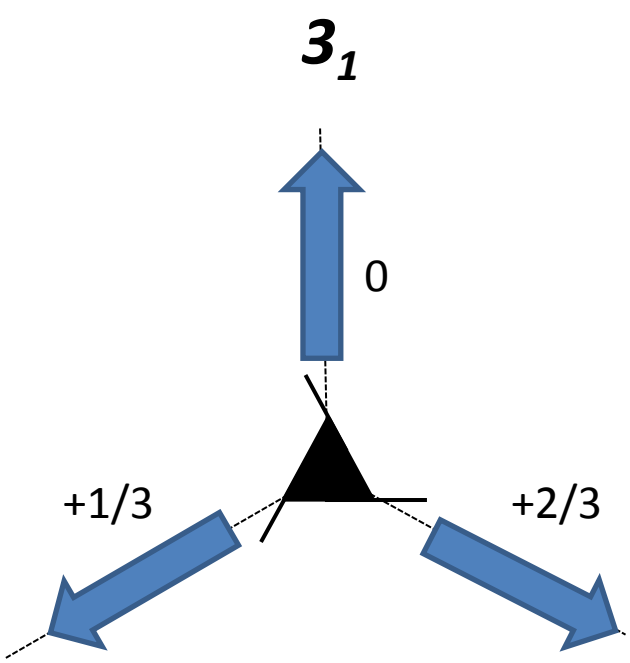


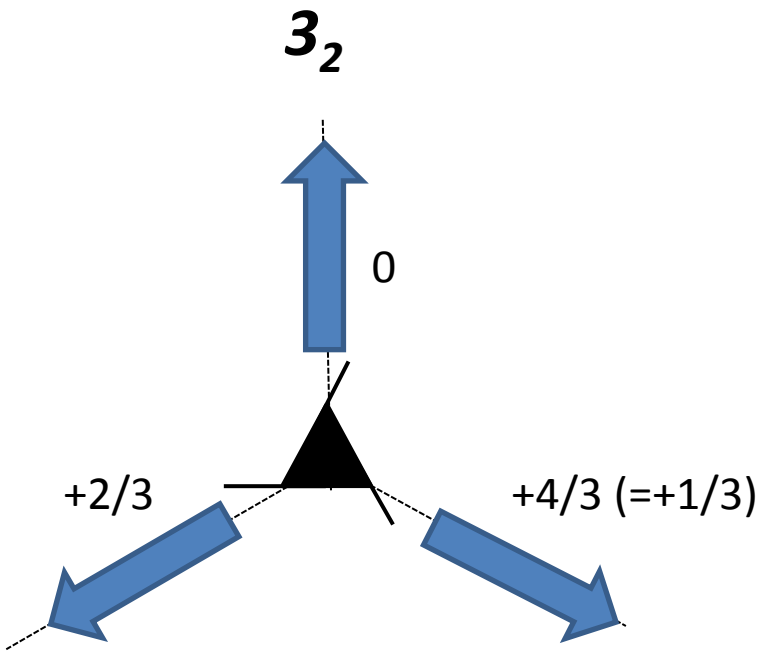
Notation for a screw axis

n_m *(n denotes rotation angle and m denotes the displacement)*

$\alpha = 360 / n$

d = a·m/n, where a is the lattice period along direction of the axis





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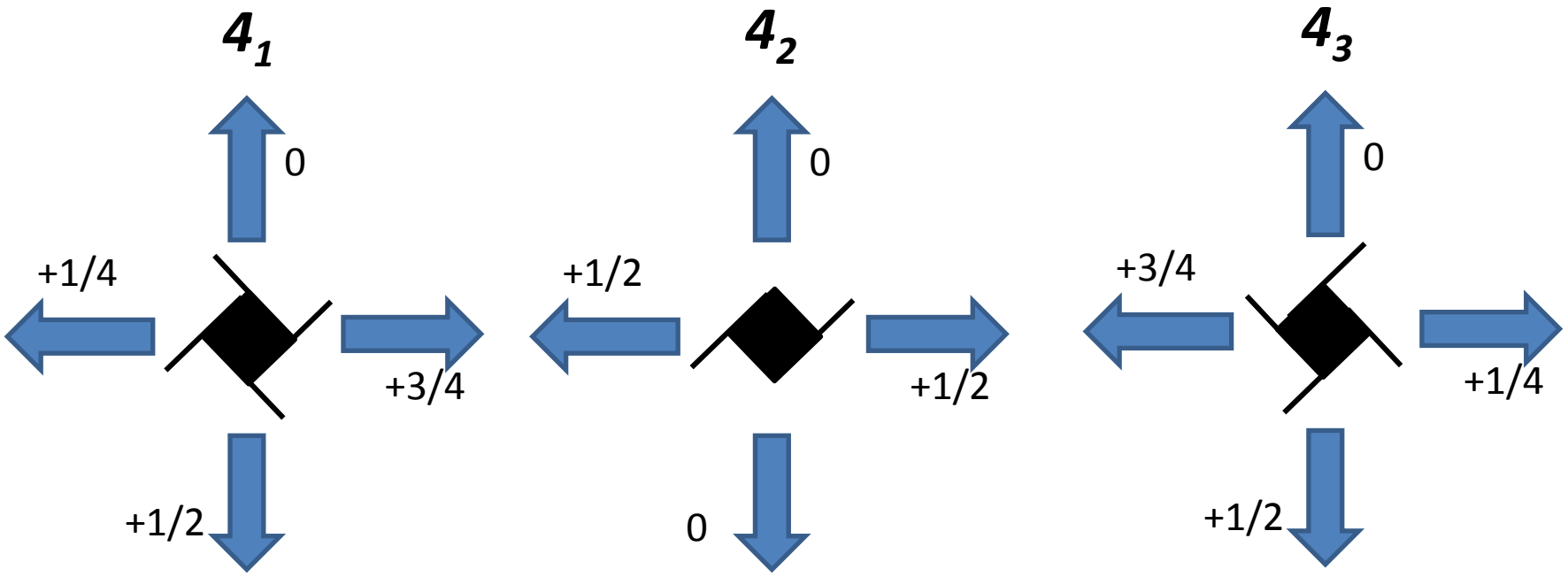

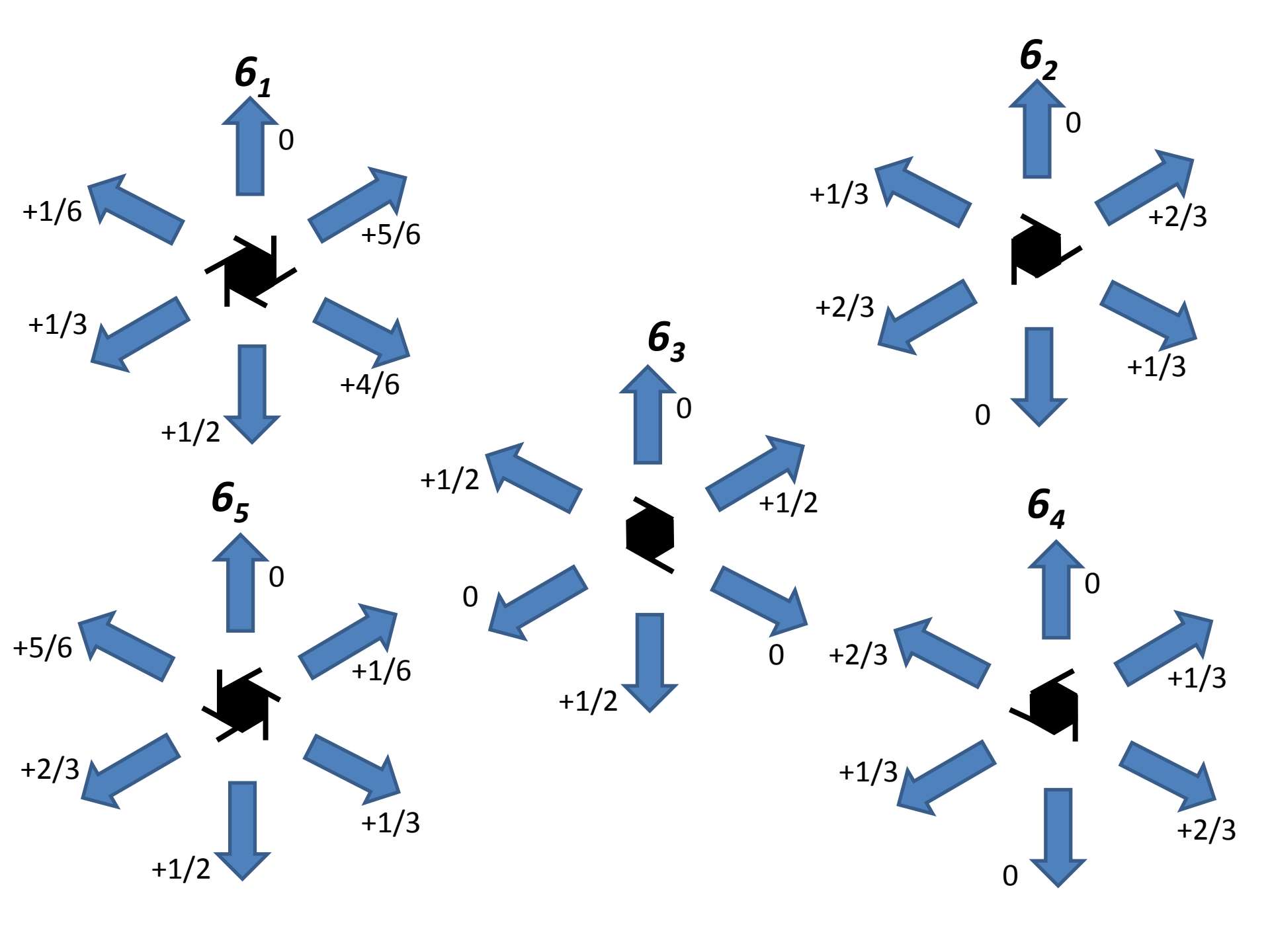
6_1
0
+1/6
+5/6
+1/3
+4/6
+1/2
6_2
0
+1/3
+2/3
+2/3
+1/3
0
6_3
0
+1/2
+1/2
0
0
+1/2
6_4
0
+2/3
+1/3
+1/3
+2/3
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6_5
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+1/6
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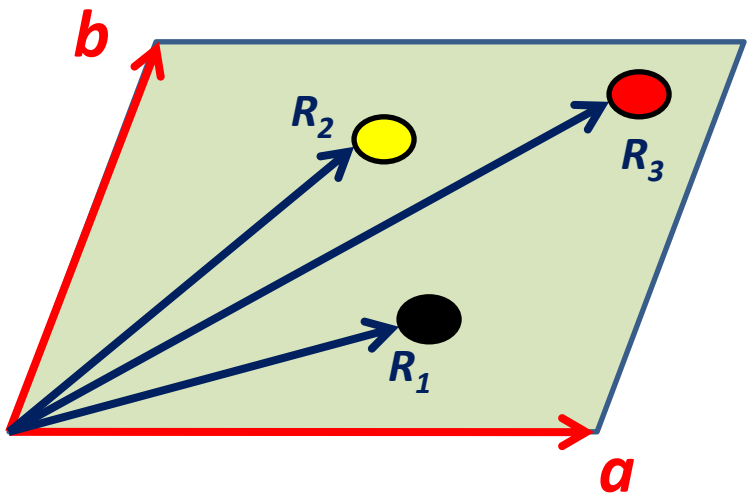
UNIT CELL and ATOMIC POSITIONS



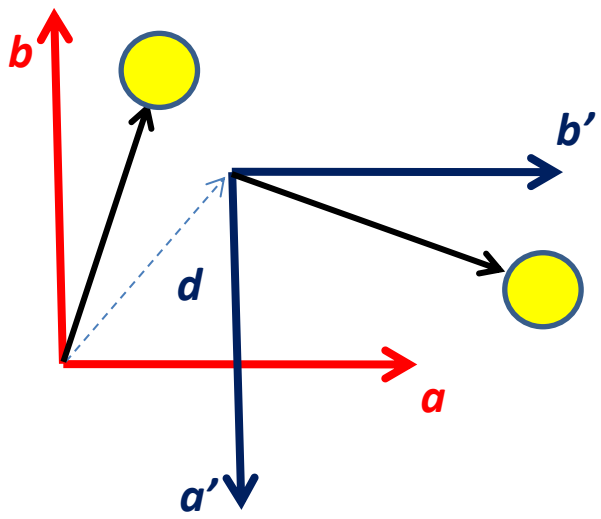
Consider a crystal lattice. According to its Bravais type we chose the conventional pair (triple) of basis vectors: ***a***,***b*** and ***c.*** The crystallographic unit cell is defined by putting atoms, molecules, etc to the sites, ***R_1 , R_2 ,..., R_n inside the parallelogram based on the vectors a, b and c.*** The site of each and every atom in the unit cell is given by the *fraction atomic positions, x, y and z.*

$$\boldsymbol{R} = x\boldsymbol{a} + y\boldsymbol{b} + z\boldsymbol{c},$$

with $0 \le x < 1,\ 0 \le y < 1,\ 0 \le z < 1$

The lattice translations are applied to each atomic positions, i.e. if there is an atom with the coordinate [x,y,z] then there is also an atom with the coordinates [x+u, y+v, z+w]. Translation [uvw] is regarded as symmetry operation

Matrix representation for symmetry operation



Any symmetry operation can be presented by the rotation matrix and displacement vector. Suppose the lattice is built on the basis vectors ***a***, ***b*** and ***c*** and the position of atoms are given by the fractional coordinates [xyz] so that ***R*** = x***a***+y***b***+z***c***. If we apply the movement related to the particular symmetry operation, the vectors a, b and c are transformed into a', b' and c' and the origin is displaced by the vector ***d***. ***The position of symmetry equivalent atom is***

$$\mathbf{R'} = x\,\mathbf{a'} + y\,\mathbf{b'} + z\,\mathbf{c'} + \mathbf{d} = x_1\,\mathbf{a} + y_1\,\mathbf{b} + z_1\,\mathbf{c}$$

$$\begin{cases} \mathbf{a}' = S_{11}\mathbf{a} + S_{21}\mathbf{b} + S_{31}\mathbf{c} \\ \mathbf{b}' = S_{12}\mathbf{a} + S_{22}\mathbf{b} + S_{32}\mathbf{c} \\ \mathbf{c}' = S_{13}\mathbf{a} + S_{23}\mathbf{b} + S_{33}\mathbf{c} \\ \mathbf{d} = d_1\,\mathbf{a} + d_2\,\mathbf{b} + d_3\,\mathbf{c} \end{cases} \longrightarrow \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} d_1 \\ d_2 \\ d_3 \end{pmatrix}$$

Rotation matrix ***Displacement vector***

Combination of symmetry operations in terms of matrices

Symmetry operation 1: $\{\boldsymbol{S_1}, \boldsymbol{d_1}\}$ $\quad \boldsymbol{R}_1 = \boldsymbol{S}_1 R_0 + \boldsymbol{d}_1$

Symmetry operation 2: $\{\boldsymbol{S_2}, \boldsymbol{d_2}\}$ $\quad \boldsymbol{R}_2 = \boldsymbol{S}_2 R_0 + \boldsymbol{d}_2$

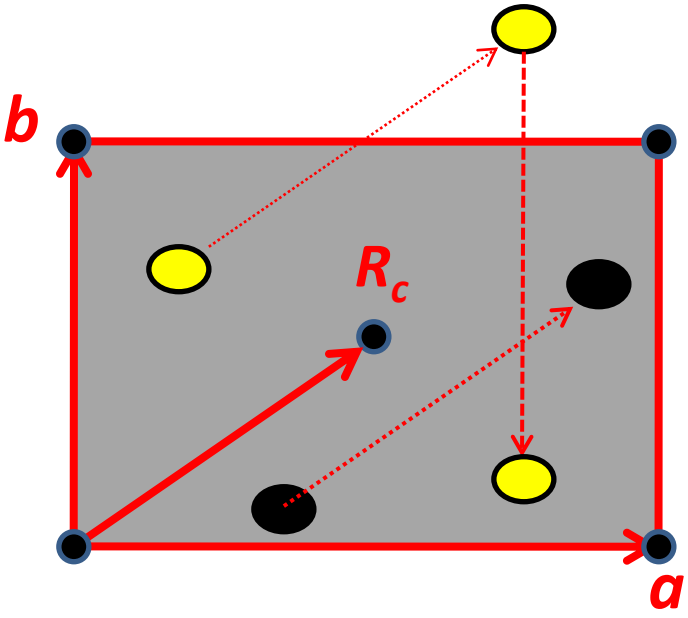
Symmetry operation 3: $\{\boldsymbol{S_1}, \boldsymbol{d_1}\}$ -> $\{\boldsymbol{S_2}, \boldsymbol{d_2}\}$

$$\boldsymbol{R_2} = \boldsymbol{S_2 R_1} + \boldsymbol{d_2} \quad = \boldsymbol{S_2 S_1 R_0} + \boldsymbol{S_2 d_1} + \boldsymbol{d_2}$$

The combination of symmetry operation is represented by the rotation matrix $\boldsymbol{S_2 S_1}$ and displacement vector $\boldsymbol{S_2 d_1 + d_2}$

For the CENTERED LATTICES.

We know that for 7 (out of 14) types of Bravais lattices the basis vectors are chosen in the way that the unit cell contains additional point. For these cases the translation by the centering vector(such as [1/2 1/2 1/2]) is also ***a symmetry operation***



Forming crystallographic unit cell:

1) $[x\ y\ z] \rightarrow [x\ y\ z] + [x_c\ y_c\ z_c]$

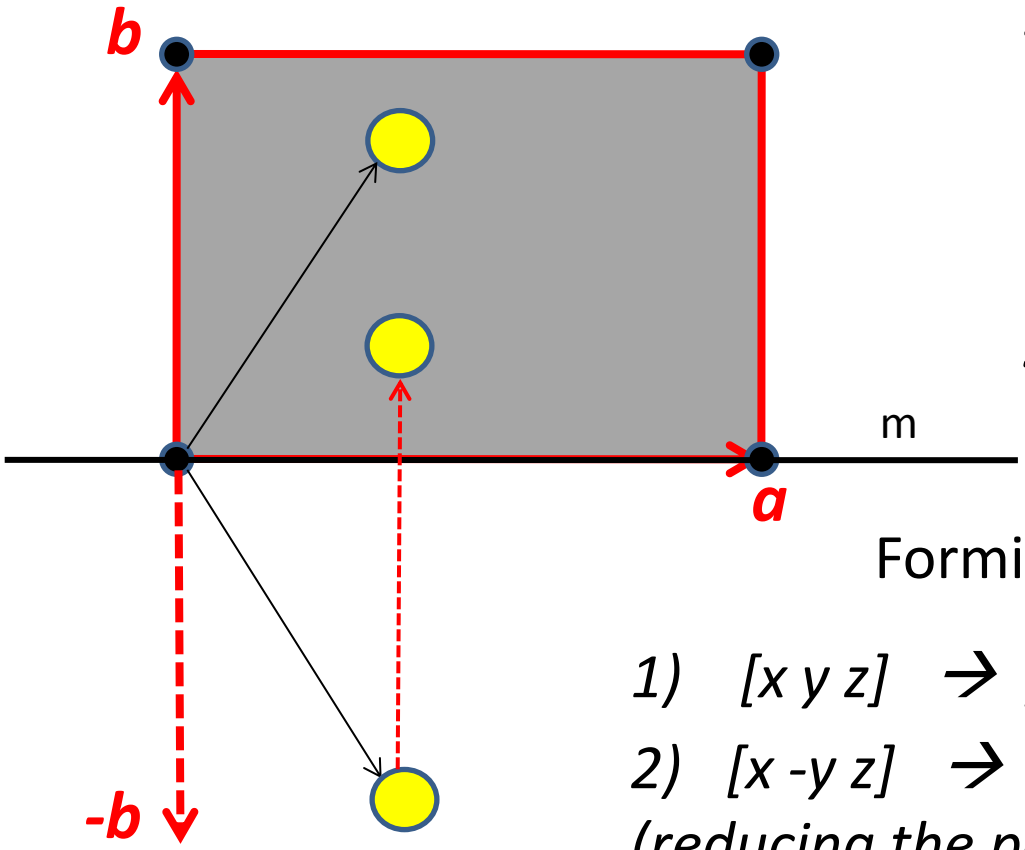
2) $[x\ y\ z] \rightarrow [x\ y\ z] + [x_c\ y_c\ z_c] + [uvw]$

(reducing the position to the crystallographic unit cell, i.e. providing $0 \le x < 1,\ 0 \le y < 1,\ 0 \le z < 1$)

Example: C - centred lattice ([0.5 0.5 0]).

Original positions	Adding centring vector	Lattice vector	The final position in the unit cell
[x y z]	*[x y z]* + R_C	A_{uvw}	[x y z] +R_C + A_{uvw}
[0 0 0]	[0.5 0.5 0]	[0 0 0]	[0.5 0.5 0]
[0.2 0.7 0.7]	[0.7 1.2 0.7]	[0 -1 0]	[0.7 0.2 0.7]
[0.6 0.4 0.2]	[1.1 0.9 0.2]	[-1 0 0]	[0.1 0.9 0.2]
[0.7 0.8 0.1]	[1.2 1.3 0.1]	[-1 -1 0]	[0.2 0.3 0.1]

Unit cell and point symmetry operations



Suppose that crystal belongs to the rectangular crystal system and has the mirror plane parallel to ***a. Then the atom is duplicated by symmetry operation***

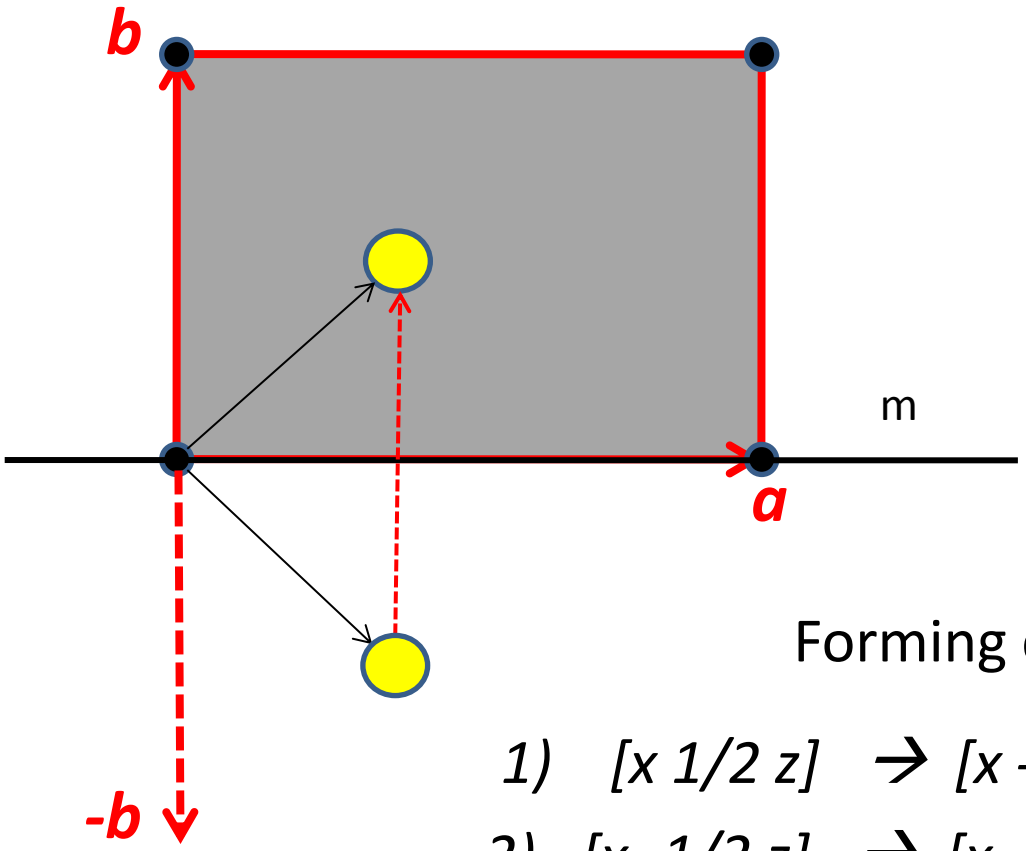
Forming crystallographic unit cell:

1) [x y z] → [x -y z]

2) [x -y z] → [x -y z] + [uvw]

(reducing the position to the crystallographic unit cell $0 \le x < 1$, $0 \le y < 1$, $0 \le z < 1$)

Special positions in the unit cell



However we can consider a special case when the initial position of an atom in the unit cell is [x, 1/2, z]. In this case

Forming crystallographic unit cell:

1) [x 1/2 z] → [x -1/2 z]

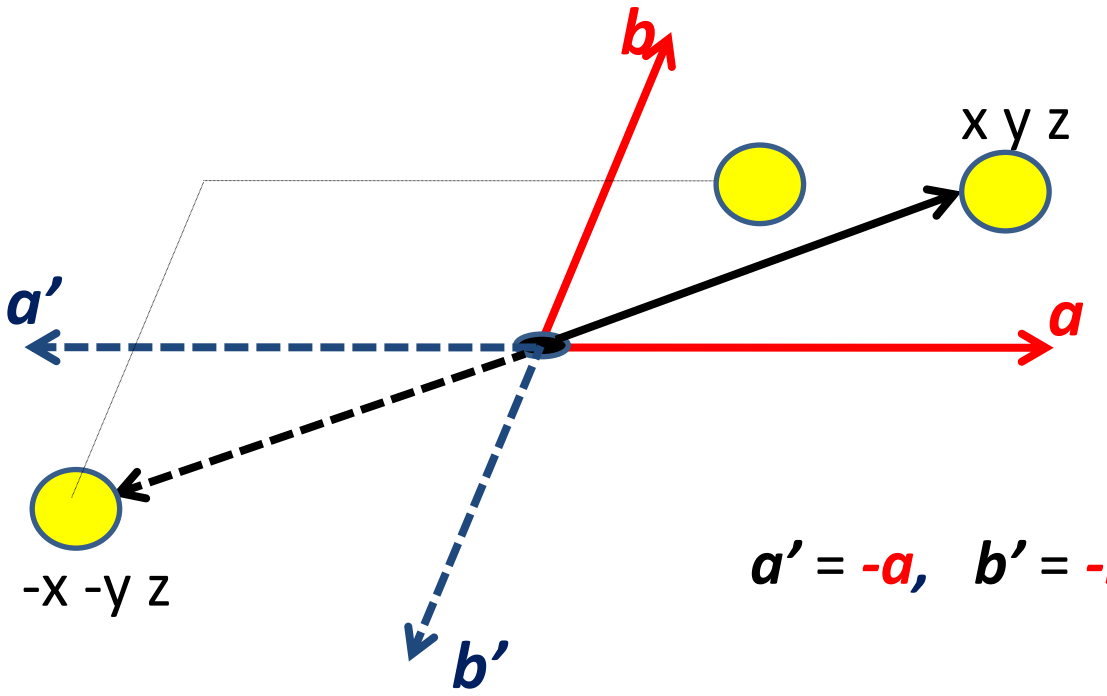
2) [x -1/2 z] → [x -1/2 z] + [010] = [x 1/2 z]

(reducing the position to the crystallographic unit cell

$0 \le x < 1, 0 \le y < 1, 0 \le z < 1$)

THE POSITION OF THE atom [x 1/2 z] is special as it is not duplicated by the symmetry operation

Mathematical description of symmetry operations. Two fold axis parallel to ***c***



After the rotations by 180 degrees the basis vectors ***a,b*** and ***c*** are transformed (***a*** → ***a'*** , ***b*** → ***b'*** ***and c*** → ***c'***) so that

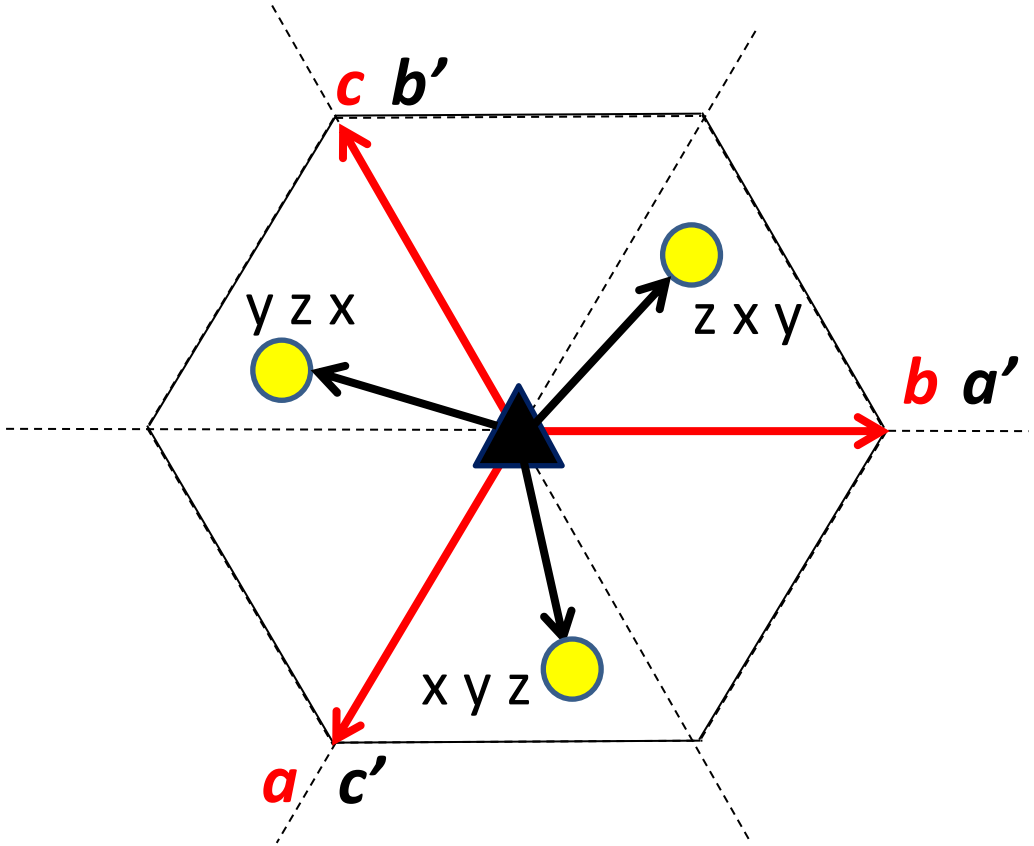
a' = ***-a***, ***b'*** = ***-b***, ***c'*** = ***c***

The position of symmetry equivalent atom is x***a'***+y***b'***+z***c'*** = -x***a***-y***b***+z***c*** = [xyz]

2 fold rotation axis parallel to the ***c*** (provided ***a*** and ***b*** is perpendicular to ***c***) gives two symmetry equivalent atoms

1) x y z 2) -x -y z

Mathematical description of symmetry operations.
Three fold axis parallel to ***c (Rhombohedral setting)***



After the rotations by 120 degrees the basis vectors ***a,b*** and ***c*** are transformed (***a*** → ***a'*** , ***b*** → ***b'*** ***and c*** → ***c'***) so that

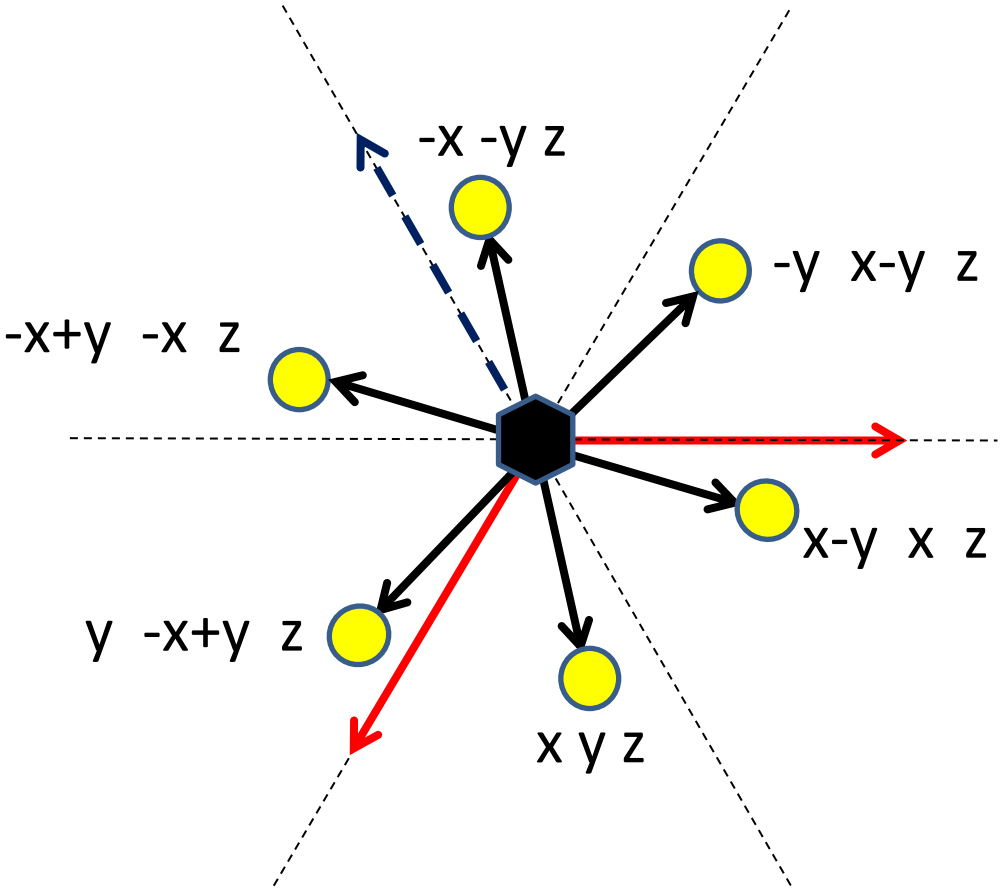
a' = ***b,*** ***b'*** = ***c,*** ***c'*** = ***a***

The position of symmetry equivalent atom should be x***a'***+y***b'***+z***c'*** = x***b***+y***c***+z***a*** = [zxy]

3 fold rotation axis parallel to the [111] gives three symmetry equivalent atoms

1) x y z 2) z x y 3) y z x

Mathematical expression for the symmetry operations: 6 fold

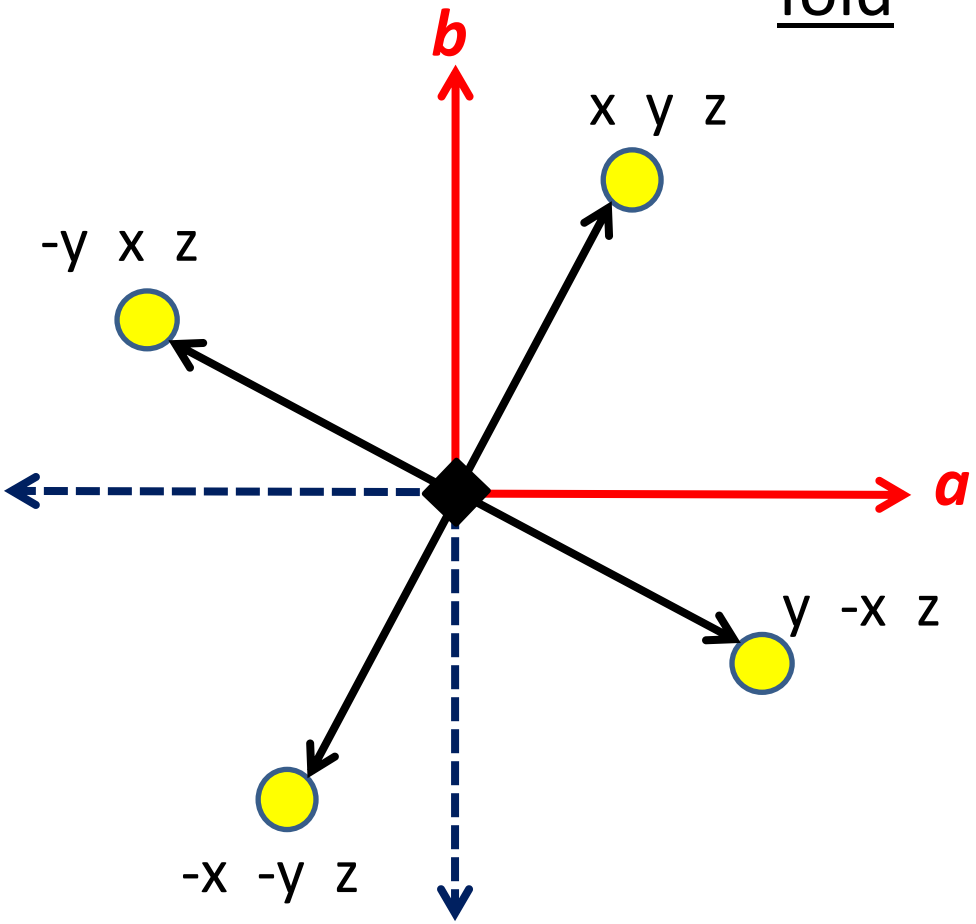


6 fold rotation axis parallel to the ***c*** gives six symmetry equivalent atoms

1) x y z 2) x-y x z 3) -y x-y z

4) -x -y z 5) -x+y -x z 6) y -x+y z

Mathematical expression for the symmetry operations: 4 fold



4 fold rotation axis parallel to the ***c*** (provided ***a*** and ***b*** is perpendicular to ***c***) gives four symmetry equivalent atoms

1) x y z 2) -x -y z 3) -y x z 4) y -x z

SUMMARY OF MATHEMATICAL REPRESENTATION OF SYMMETRY

n	*Orientation*	*The list of atomic positions*
 *2*	*|| **c***	*1) x y z 2) -x -y z*
 *3*	*|| **a+b+c***	*1) x y z 2) z x y 3) y z x*
 *4*	*|| **c***	*1) x y z 2) -x -y z* *3) -y x z 4) y -x z*
 *6*	*|| **c***	*1) x y z 2) x-y x z 3) -y x-y z* *4) -x -y z 5) -x+y -x z 6) y -x+y z*

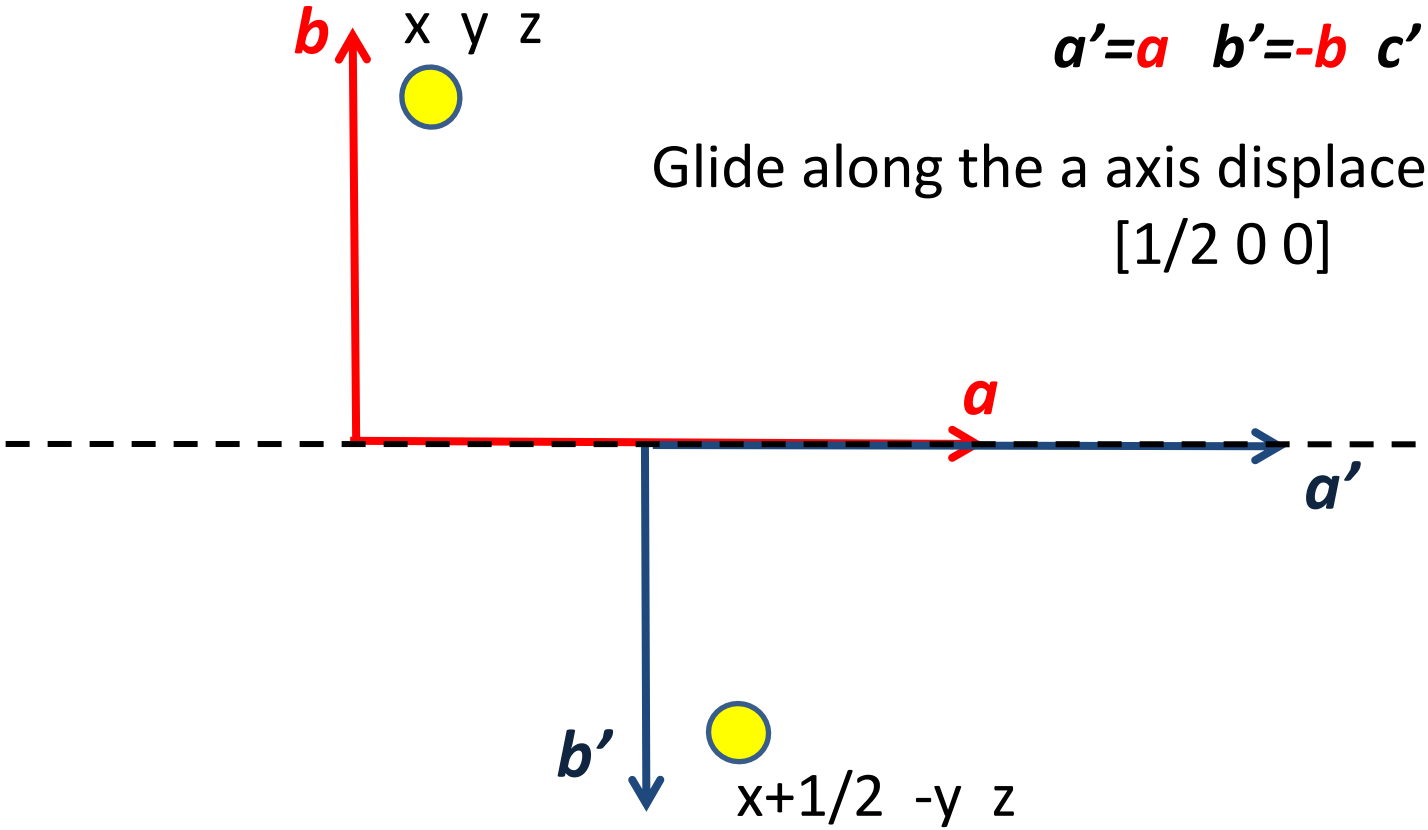
The reduction to the crystallographic unit cell, i.e. adding the lattice vector [uvw] or centering lattice vector (e.g [1/2 1/2 1/2]) should be performed after the above transformation

Mathematical expression for glide plane (a)

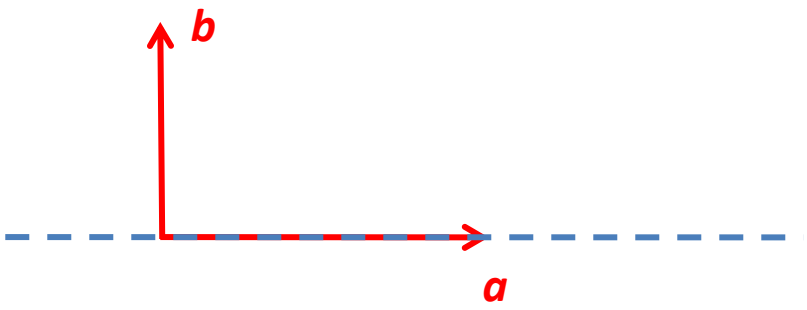
After the reflection in the plane perpendicular to ***b*** the basis vectors ***a, b*** and ***c*** are transformed (***a*** → ***a'*** , ***b*** → ***b'*** ***and c*** → ***c'***) so that

a'=a b'=-b c' = c

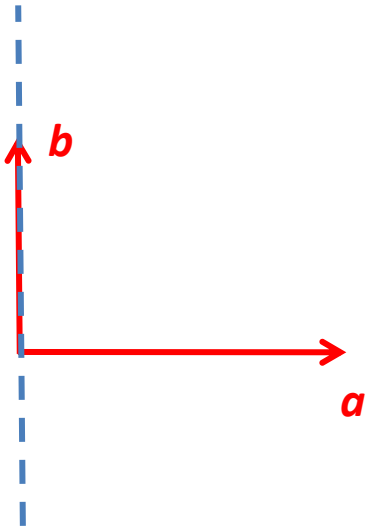
Glide along the a axis displaces the origin by [1/2 0 0]



Example: matrix representation of glide planes



$$\mathbf{S} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{d} = \begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix}$$



$$\mathbf{S} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{d} = \begin{pmatrix} 0 \\ 1/2 \\ 0 \end{pmatrix}$$