Screw axes and glide planes

UNIVERSITÉ DE LORRAINE

CRM^2 Cristallographie, Résonance Magnétique et Modélisations

cnrs

iJB Institut Jean Barriol

Didactic material for the MaThCryst schools

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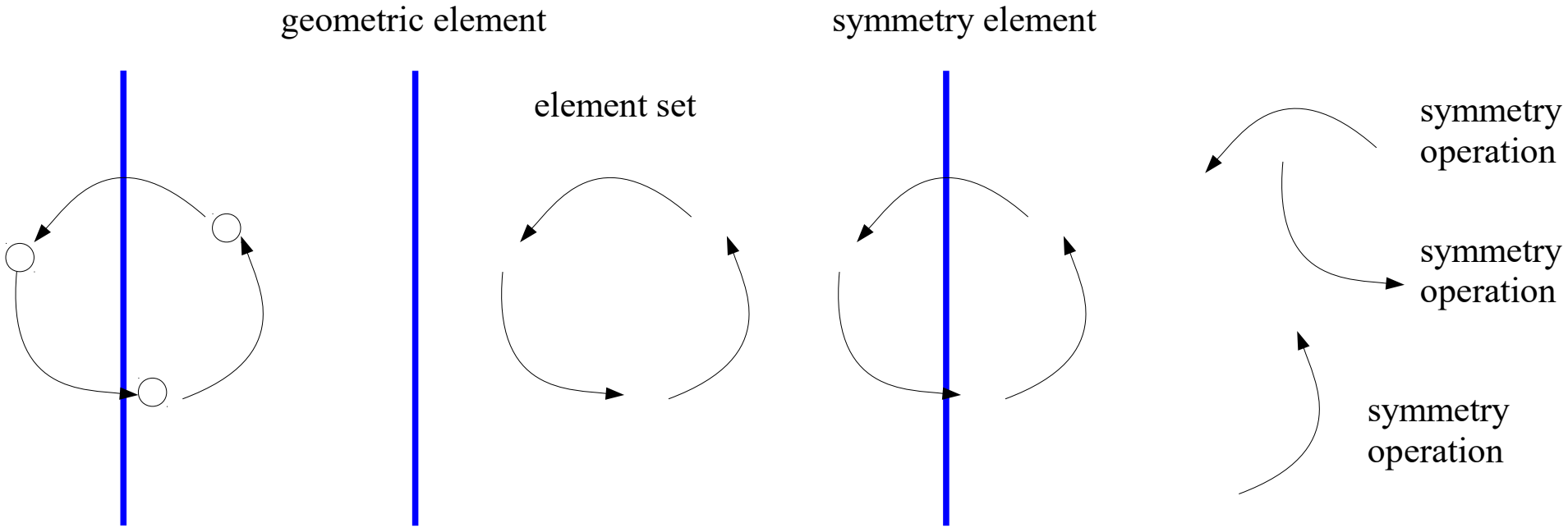
MaThCryst IUCr

Elements and operations

- **geometric element** : the point, line or plane left invariant by the symmetry operation.
- **symmetry element**: the geometric element defined above together with the set of operations (called **element set**) that leave in invariant.
- **symmetry operation** : an isometry that leave invariant the object to which it is applied.



The operation that share a given geometric element differ by a lattice vector. The one characterized by the shortest vector is called **defining operation**.

Finding the geometric element

- Remove the intrinsic translation part (screw or glide component).
- Impose that the coordinates of the geometric element are fixed by the operation.

$$\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & \bar{1} & 1/2 \end{array}\right)$$

Intrinsic part: screw component

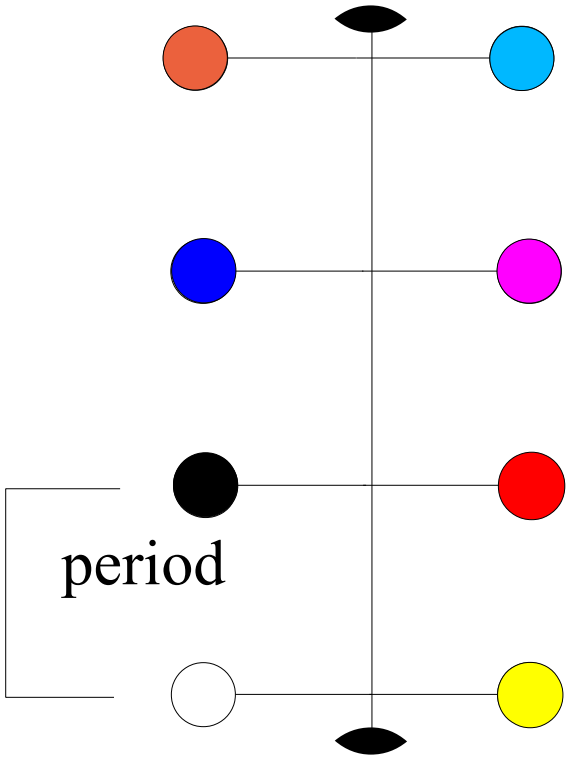
Location part: the element does not pass through the origin

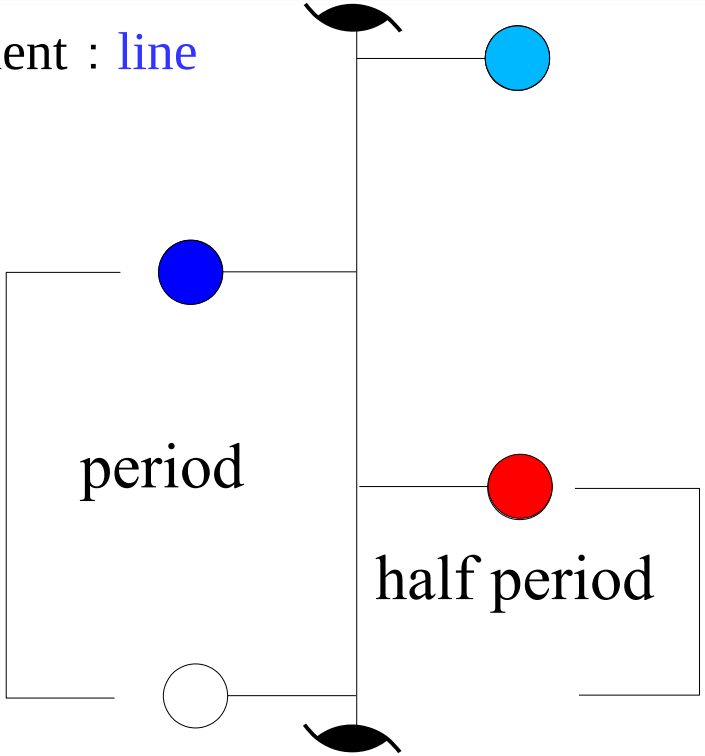
Linear part: twofold rotation about [010]

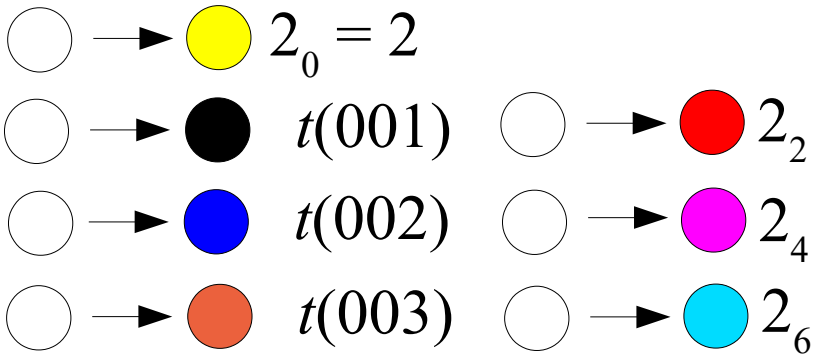
$$\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & 1/2 \end{array}\right)\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} \qquad \begin{cases} -u = u \\ v = v \\ -w + 1/2 = w \end{cases} \qquad \begin{cases} u = 0 \\ \forall v \\ w = 1/4 \end{cases} \qquad 0,y,¼$$

Screw axes n_p (screw component: p/n)

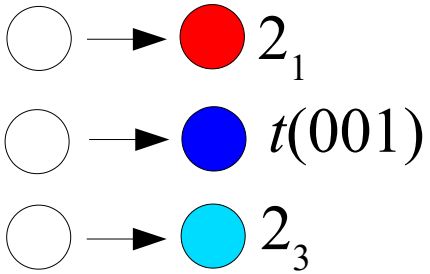
Geometric element : line







Defining operation : twofold rotation
Symmetry element : rotation axis



Defining operation : twofold screw rotation
Symmetry element : screw axis

http://dx.doi.org/10.1002/crat.201600129
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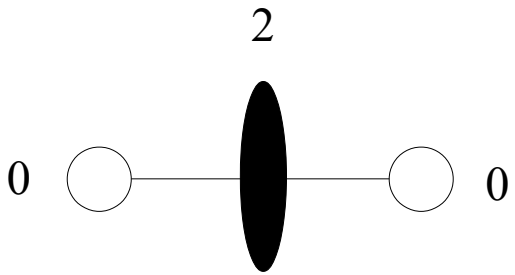
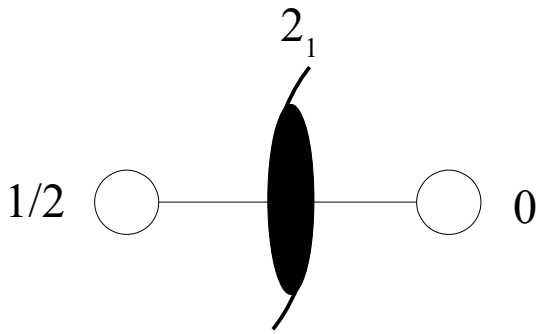
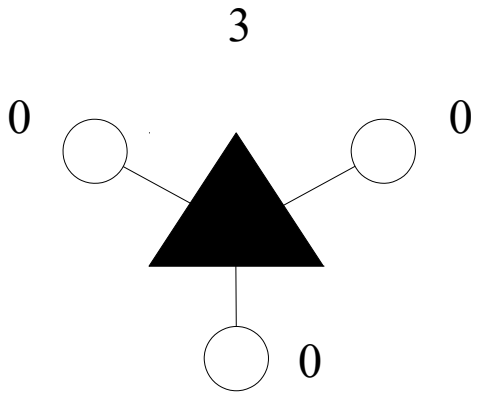
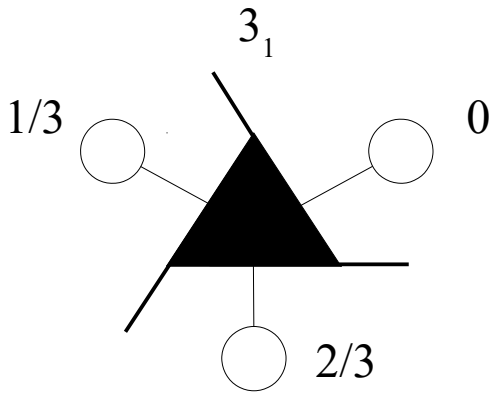
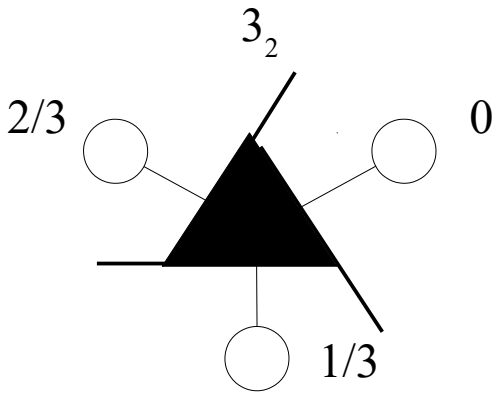
Screw axes



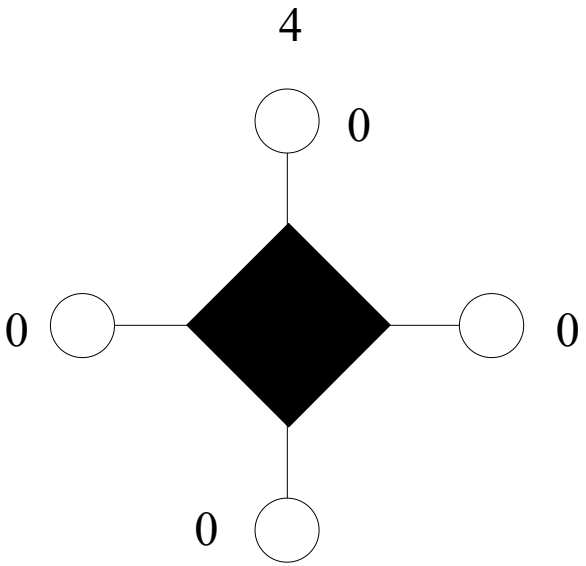


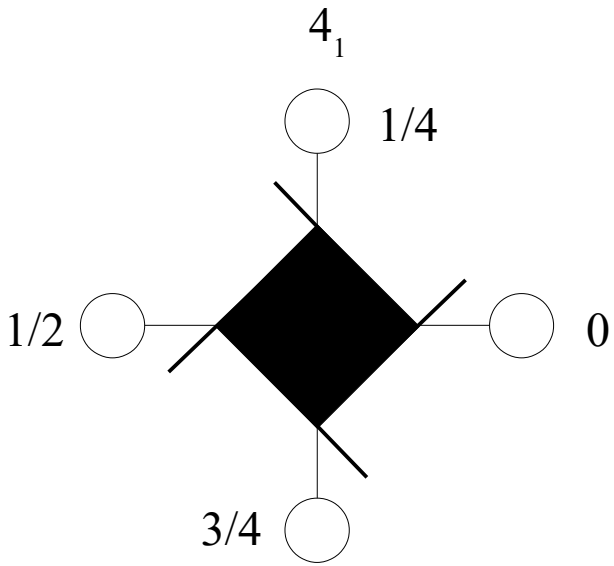


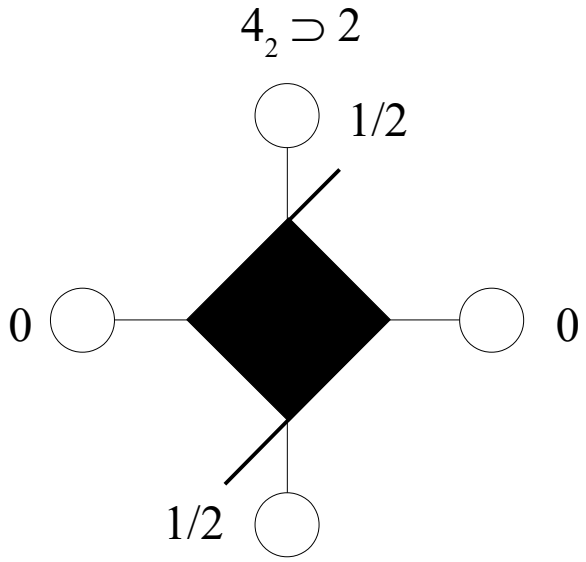


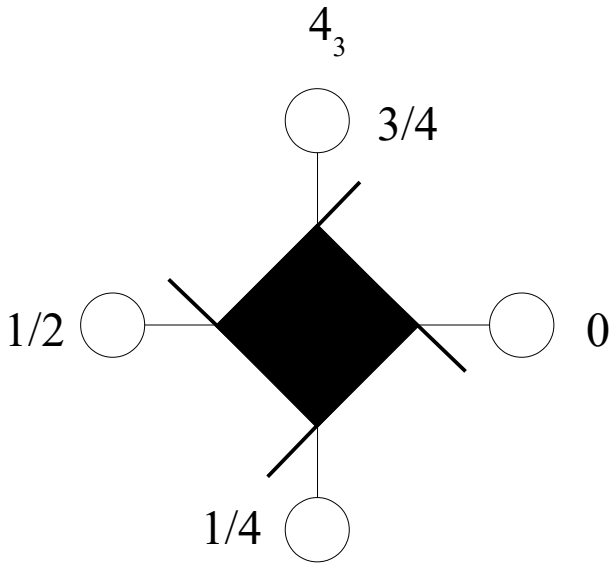


Screw axes



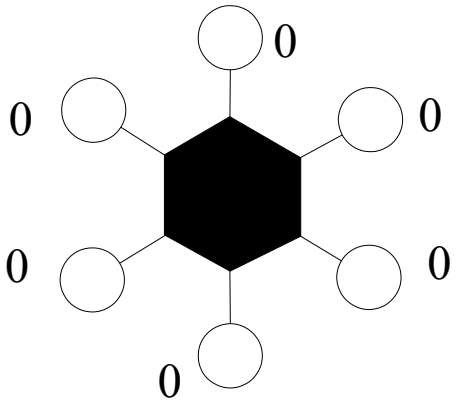




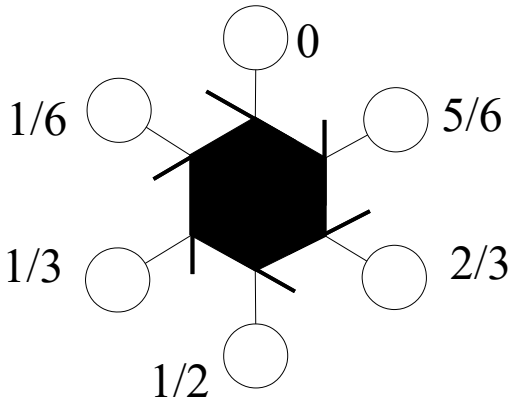


Screw axes

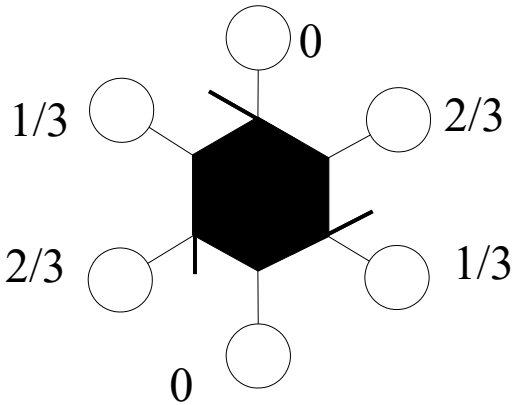
6



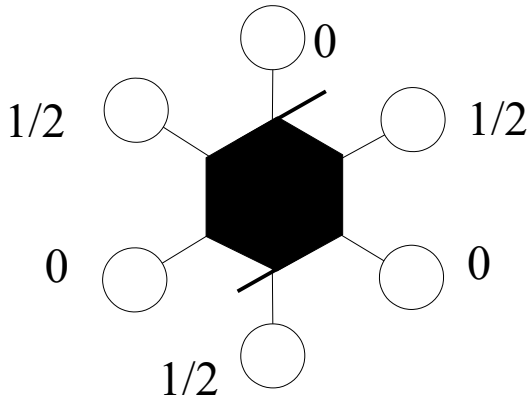
6_1



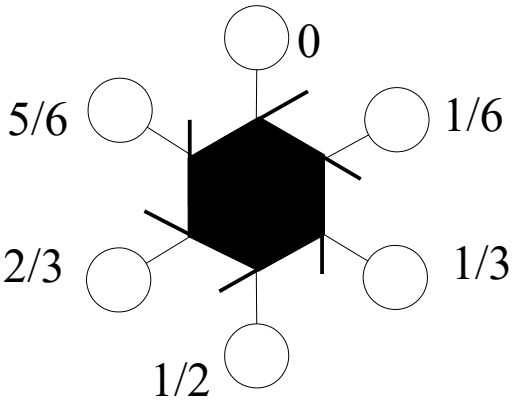
$6_2 \supset 2$



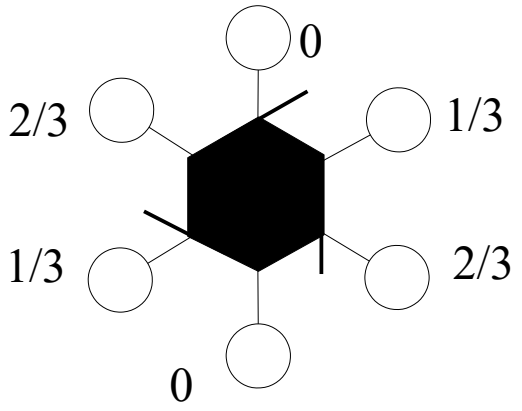
$6_3 \supset 3$



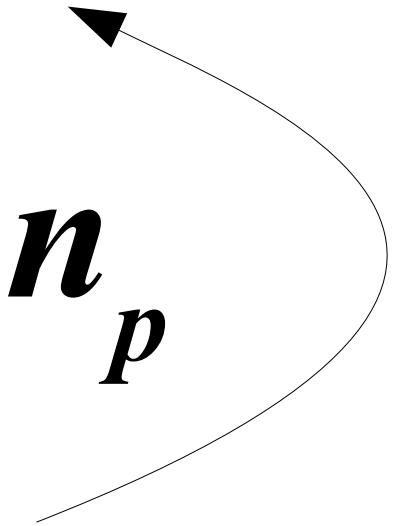
6_5

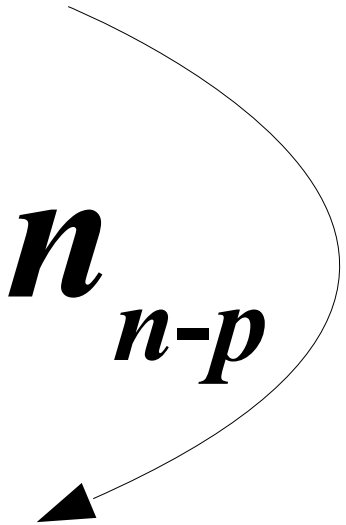


$6_4 \supset 2$



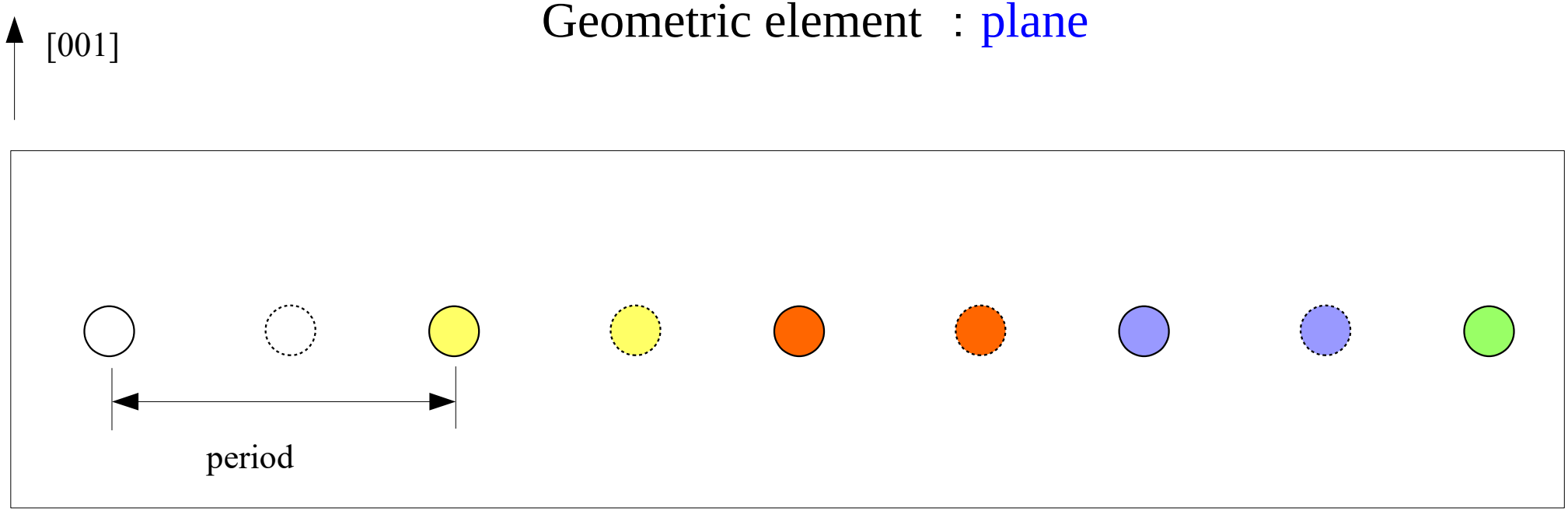
Screw axes





Glide planes *g*

Geometric element : plane



g (½ ½,0) *x*,*x*,*z*

g (3/2,3/2,0) *x*,*x*,*z*

g (5/2,5/2,0) *x*,*x*,*z*

g (7/2,7/2,0) *x*,*x*,*z*

t(1,1,0)

t(2,2,0)

t(3,3,0)

t(4,4,0)

Special cases

g (0,0,0): *m*

g (½,0,0): *a*

g (0,½,0): *b*

g (0,0,½): *c*

g (half-diagonal): *n*

g (quarter-diagonal): *d*

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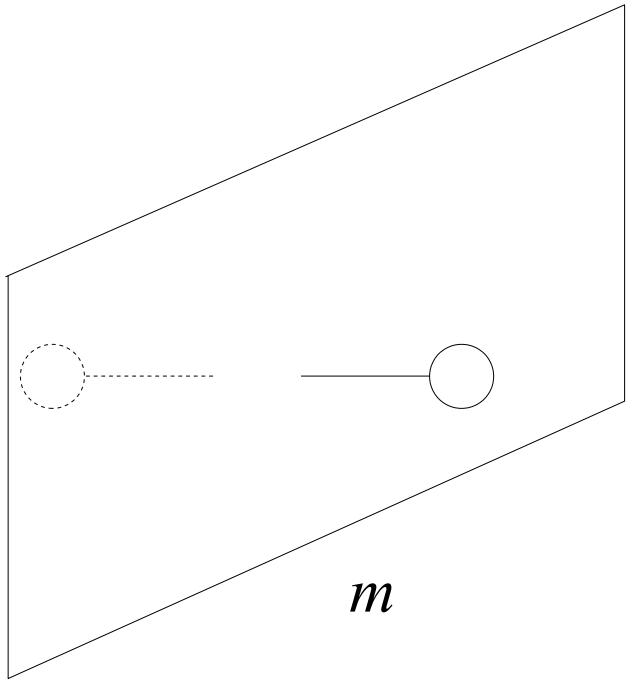
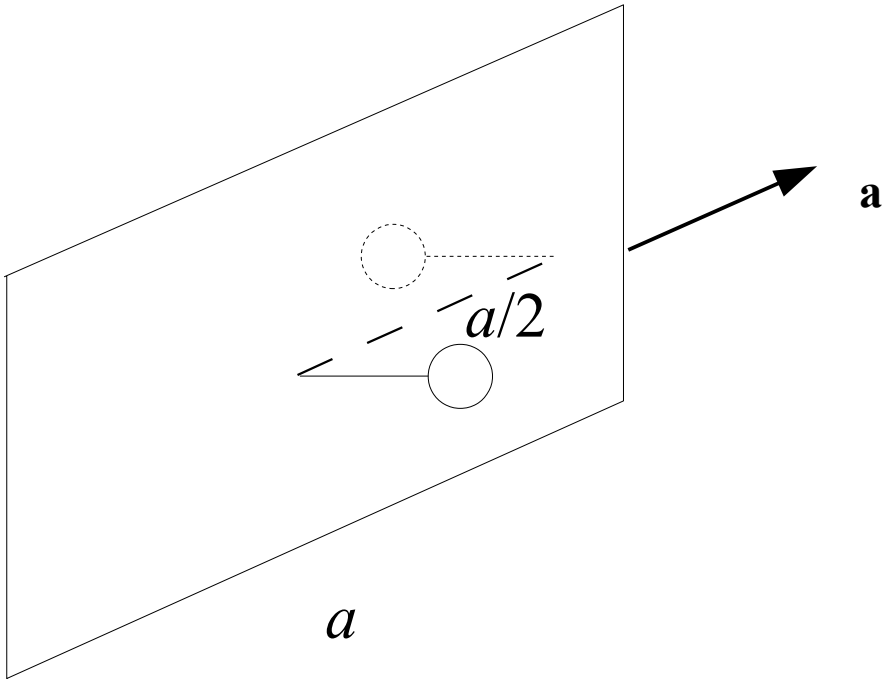
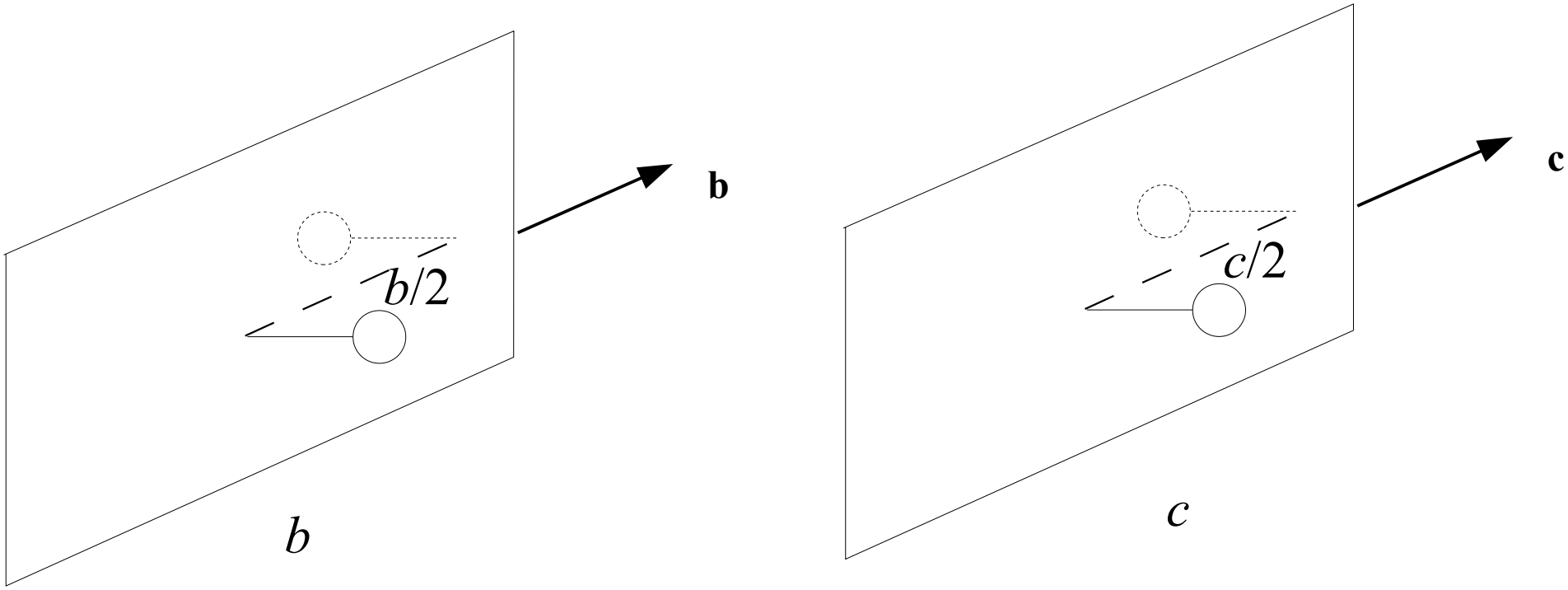
Glide planes



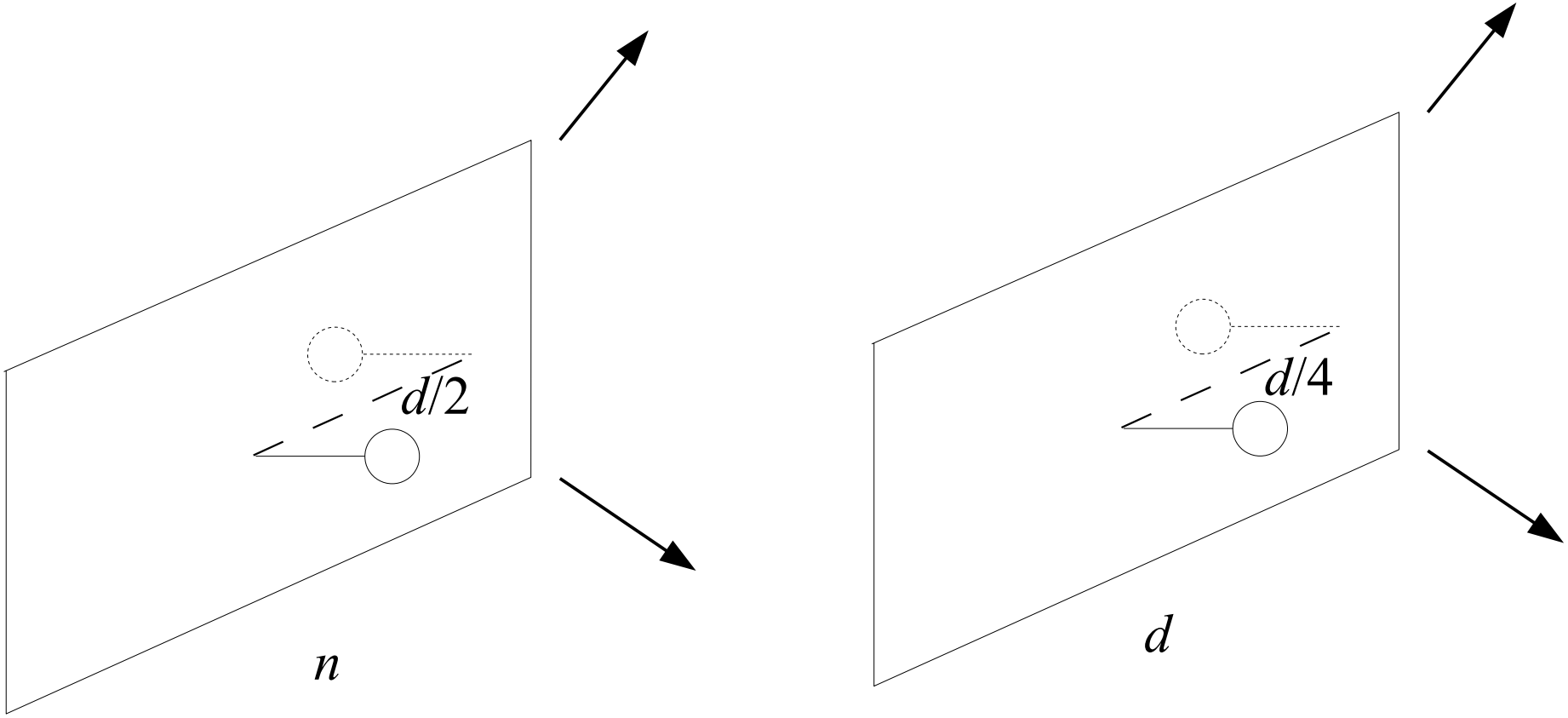


Glide planes



Diamond structure glide plane

Glide planes

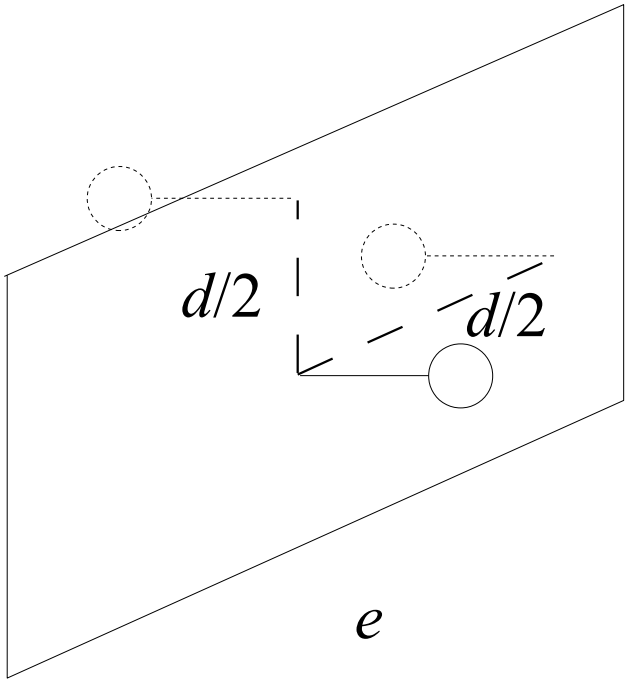


dia**g**o**n**al

Diamond structure glide plane

2D glide line; 3D glide plane with “unusual' glide

Glide planes



How can we have a glide of ¼ if the reflection is an operation of order 2 ?

If the unit cell is centred !

Vector centring the unit cell, with a norm $p/2$