Symmetry

- Repetition

1. Lattice translation- three non-coplanar lattice translation

space lattice

2. Rotation (회전)

3. Reflection (반사)

4. Inversion (반전)



Symmetry Aspects of M. C. Escher's Periodic Drawings



plate 9

Fig. 1.1. Pattern based on a fourteenth-century Persian tiling design.



http://www.iucr.ac.uk/

Fig. 1.2. A teacup, showing its mirror plane of symmetry. (After L. S. Dent Glasser, Crystallography & its applications: Van Nostrand Reinhold, 1977.)



http://www.iucr.ac.uk/

Fig. 1.3. Some symmetry elements, represented by human figures. (a) Mirror plane, shown as dashed line, in elevation and plan. (b) Twofold axis, lying along broken line in elevation, passing perpendicularly through clasped hands in plan. (c) Combination of twofold axis with mirror planes; the position of the symmetry elements given only in plan. (d) Threefold axis, shown in plan only. (e) Centre of symmetry (in centre of clasped hands). (f) Fourfold inversion axis, in elevation and plan, running along the dashed line and through the centre of the clasped hands.

(After L. S. Dent Glasser, Chapter 19, The Chemistry of Cements: Academic Press, 1964.)











Symmetry

- * All repetition operations are called **symmetry operations**. Symmetry consists of the repetition of a pattern by the application of specific rules.
- * When a symmetry operation has a locus, that is a point, or a line, or a plane that is left unchanged by the operation, this locus is referred to as the symmetry element.
- * Symmetry operation symmetry element reflection mirror plane rotation rotation axis inversion inversion center (center of symmetry)

- general plane lattice

180° rotation about the central lattice point A- coincidence - 2 fold rotation axis symbol: 2, • \rightarrow $n = \frac{360^{\circ}}{\phi} = \frac{2\pi}{\phi}$ normal or parallel to plane of paper



-n-fold axis $n = \frac{360^{\circ}}{\phi} = \frac{2\pi}{\phi}$ \$\overline\$ iminimum angle required to reach a position indistinguishable -n > 2 produce at least two other points lying in a plane normal to it - three non-colinear points define a lattice plane - fulfill the conditions for being a lattice plane (translational periodicity)







II-V and III-IV parallel but not equal or integral ratio

* In space lattices and consequently in crystals, only 1-, 2-, 3-,

4-, and 6-fold rotation axes can occur.



http://jcrystal.com/steffenweber/JAVA/jtiling/jtiling.html



http://jcrystal.com/steffenweber/JAVA/jtiling/jtiling.html



– limitation of ϕ set by translation periodicity



- Matrix representation of rotation in Cartesian coordinate



$$R(2_{z}^{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(3_{z}^{1}) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(3_{z}^{2}) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(4_{z}^{1}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R(4_{z}^{2}) = R(2_{z}^{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R(4_{z}^{3}) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(4_z^1) \bullet R(4_z^2) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = R(4_z^3)$$

- hexagonal coordinate





Standard (0001) projection (hexagonal, c/a=1.86)

$$\begin{array}{ll} x_2 = -y_1 & x_3 = -x_1 + y_1 \\ y_2 = x_1 - y_1 & y_3 = -x_1 \\ z_2 = z_1 & x_3 = z_1 \end{array} \quad R(3_z^1) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R(3_z^2) = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



* Cartesian coordinate

$$R(3_{z}^{1}) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0\\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0\\ 0 & 0 & 1 \end{pmatrix}$$

Reflection

- reflection, a plane of symmetry or a mirror plane, m, [, Γ





Inversion

- inversion, center of symmetry or inversion center, $\overline{1}$ \circ



Inversion



Inversion centre

http://www.gh.wits.ac.za/craig/diagrams/

Compound Symmetry Operation

- link of translation, rotation, reflection, and inversion operation

- -compound symmetry operation two symmetry operation in sequence as a single event
- combination of symmetry operations two or more individual symmetry operations are combined which are themselves symmetry operations



Compound Symmetry Operation

Table 5.1. Compound symmetry operations of simple operations. The corresponding symmetry elements are given in round brackets

	Rotation	Reflection	Inversion	Translation
Rotation	×	Roto- reflection	Roto- inversion	Screw rotation
Reflection	(Roto- reflection axis)	×	2-fold rotation	Glide reflection
Inversion	(Roto- inversion axis)	(2-fold rotation axis)	×	Inversion
Translation	(Screw axis)	(Glide plane)	(Inversion centre)	×

 \bigcirc

-compound symmetry operation of rotation and inversion



 $\overline{1} \equiv inversion centre$

- down, left
- O up, right

 $\overline{2}(\equiv m)$



















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 $\overline{1} \equiv$ inversion center, $\overline{2} \equiv m$, $\overline{3} \equiv 3 + \overline{1}$, $\overline{4}$ implies 2, $\overline{6} \equiv 3 \perp m$,

only rotoinversion axes of odd order imply the presence of an inversion center

Rotoreflection



- The axes *n* and *n*, including 1 and *m*, are called point-symmetry element, since their operations always leave at least one point unmoved



- a mirror plane is added normal to the rotation axis, $\frac{X}{m}$



- a mirror plane is added normal to the rotation axis, Xm



- a mirror plane is added normal to the rotation axis, Xm

 $4m (\equiv 4mm)$



 $6m (\equiv 6mm)$



Simultaneous Rotational Symmetry



Crystal could, conceivably,
be symmetrical with respect to
many different intersection n fold axis

Two rotations about intersecting axes

 \rightarrow inevitably create a third rotation equivalent to the combination



 $A_{\alpha} \cdot B_{\beta} = C_{\gamma}$

Rotation around A axis to α

By the vector notation ;

$$\vec{s} + \vec{t} = \vec{R}$$

or $\vec{s} + \vec{t} - \vec{R} = 0$

 $A_{\alpha} \cdot B_{\beta} \cdot C_{-\gamma} = 1$ (identical operation)



The combined motions of A α and B β have the following effect :

- 1 : A α brings C to C'
- **2** : $B\beta$ restores C' to C

Thus, the combination of rotations A and B leaves C unmoved.

Therefore, if there is a motion of points on the sphere due to $A\alpha$ and $B\beta$, it must be a rotation about an axis OC

To calculate ;

 $1: A\alpha \text{ leaves } A \text{ unmoved}$

 $2: B\beta$ moves A to A

Now consider $\triangle BA'C$

 $\angle ABC = \angle A'BC = \beta/2$

AB = A'B

 $\therefore \Delta ABC = \Delta A'BC$

 $\therefore \angle ACB = \angle A'CB = \gamma/2$

From the law of cosines $\cos w = \cos u \cos v + \sin u \sin v \cos W$



since	$u = 180^{\circ} - U$	$U = 180^{\circ} - u$
	$v = 180^{\circ} - V$	$V = 180^{\circ} - v$
	$w = 180^{\circ} - W$	$W = 180^{\circ} - w$

 $\cos(180^{\circ} - W) = \cos(180^{\circ} - U)\cos(180^{\circ} - V)$ $+ \sin(180^{\circ} - U)\sin(180^{\circ} - V)\cos(180^{\circ} - w)$ $\therefore -\cos W = \cos U \cos V - \sin U \sin V \cos w$ $or \quad \cos W = -\cos U \cos V + \sin U \sin V \cos W$

 $\therefore \cos w = \frac{\cos W + \cos U \cdot \cos V}{\sin U \sin V}$

Data for crystallographic solutions of

 $\cos w = \frac{\cos W + \cos U \cos V}{\sin U \sin V}$

Axis at A, B, or C	Throw of axis, α, β, or γ	U (=α/2) V(= β/2) or W(= γ/2)	cos U, V, W	sin U, V, W
1-fold	360°	180°	-1	0
2-fold	180°	90°	0	1
3-fold	120°	60°	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$
4-fold	90°	45°	$\frac{1}{\sqrt{2}}$	$\frac{\overline{1}}{\sqrt{2}}$
6-fold	60°	30°	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$

Combinatio	on Form for first two rotations		cos w		w		
222		$\frac{0+0}{1}$	= 0		90°	. 246]
223		$\frac{\frac{1}{2}+0}{1}$	$=\frac{1}{2}$		60°	266	-
224	$\frac{\cos W + 0 \cdot 0}{1 \cdot 1}$	$\frac{\frac{1}{\sqrt{2}}+0}{\frac{1}{1}}$	$=\frac{1}{\sqrt{2}}$		45°	333	
226		$\frac{\frac{\sqrt{3}}{2}+0}{l}$	$=\frac{\sqrt{3}}{2}$	ø	30°	<i></i> 334	
233		$\frac{\frac{1}{2}+0}{\frac{\sqrt{3}}{2}}$	$=\frac{1}{\sqrt{3}}$		54° 44′	336	
234	$\frac{\cos W + 0 \cdot \frac{1}{2}}{1 \cdot \frac{\sqrt{3}}{2}}$	$\frac{\frac{1}{\sqrt{2}} + 0}{\frac{\sqrt{3}}{2}}$	$=\frac{2}{\sqrt{6}}$		35° 16'	344	
236		$\frac{\frac{\sqrt{3}}{2}+0}{\frac{\sqrt{3}}{2}}$	- [0,	346	

nbination	Form for first two rotations		cos w	w
244	$\cos W + 0 \cdot \frac{1}{\sqrt{2}}$	$\frac{\frac{1}{\sqrt{2}} + 0}{\frac{l}{\sqrt{2}}}$	- i	0.
246	$1 \cdot \frac{1}{\sqrt{2}}$	$\frac{\frac{\sqrt{3}}{2} \div 0}{\frac{1}{\sqrt{2}}}$	$=\frac{\sqrt{6}}{2}>1$	-
266	$\frac{\cos W + 0 \cdot \frac{\sqrt{3}}{2}}{1 \cdot \frac{1}{2}}$	$\frac{\frac{\sqrt{3}}{2} \div 0}{\frac{1}{2}}$	$=\sqrt{3}$ > 1	_
333)		$\frac{\frac{1}{2} + \frac{1}{4}}{\frac{2}{4}}$	- 1	0.
ari 334	$\frac{\cos W + \frac{1}{2} \cdot \frac{1}{2}}{\frac{\sqrt{3}}{2} \cdot \frac{\sqrt{3}}{2}}$	$\frac{\frac{1}{\sqrt{2}} + \frac{1}{4}}{\frac{3}{4}}$	$=\frac{2\sqrt{2}+1}{3} > 1$	-
336		$\frac{\frac{\sqrt{3}}{2} + \frac{1}{4}}{\frac{3}{4}}$	$=\frac{2\sqrt{3}+1}{3}>1$	·
344	$\cos \mathcal{W} + \frac{1}{2} \cdot \frac{l}{\sqrt{2}}$	$\frac{\frac{1}{\sqrt{2}} + \frac{1}{2\sqrt{2}}}{\frac{\sqrt{3}}{2\sqrt{2}}}$	$=\frac{3}{\sqrt{3}}>1$	-
346	$\frac{\sqrt{3}}{2} \cdot \frac{1}{\sqrt{2}}$	$\frac{\frac{\sqrt{3}}{2} + \frac{1}{2\sqrt{2}}}{\frac{\sqrt{3}}{2\sqrt{2}}}$	$=\frac{\sqrt{6}+1}{\sqrt{3}}>1$	-

Combination	Form for first two rotations		cos w	w
366	$\frac{\cos W + \frac{1}{2} \cdot \frac{\sqrt{3}}{2}}{\frac{\sqrt{3}}{2} \cdot \frac{1}{2}}$	$\frac{\frac{\sqrt{3}}{2} + \frac{1}{2} \cdot \frac{\sqrt{3}}{2}}{\frac{1}{2} \cdot \frac{\sqrt{3}}{2}}$	$=\frac{1+\frac{1}{2}}{\frac{1}{2}}=3$	_
444	$\frac{\cos W + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}}{\frac{1}{1} \cdot \frac{1}{1}}$	$\frac{\frac{1}{\sqrt{2}} + \frac{1}{2}}{\frac{1}{2}}$	$=\frac{2}{\sqrt{2}}+1>1^{\circ}$	
446	$\overline{\sqrt{2}}$, $\overline{\sqrt{2}}$	$\frac{\frac{\sqrt{3}}{2} + \frac{1}{2}}{\frac{1}{2}}$	$=\sqrt{3}+1>1$	-
466	$\frac{\cos W + \frac{1}{\sqrt{2}} \cdot \frac{\sqrt{3}}{2}}{\frac{1}{\sqrt{2}} \cdot \frac{1}{2}}$	$\frac{\frac{\sqrt{3}}{2} + \frac{1}{\sqrt{2}} \cdot \frac{\sqrt{3}}{2}}{\frac{1}{\sqrt{2}} \cdot \frac{1}{2}}$	$=\sqrt{3}(\sqrt{2}+1) > 1$	_
666	$\frac{\cos W + \frac{\sqrt{3}}{2} \cdot \frac{\sqrt{3}}{2}}{1 1}$	$\frac{\frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2} \cdot \frac{\sqrt{3}}{2}}{\frac{1}{2}}$	$= 2\sqrt{3} + 3 > 1$	_



FIG. 14. The six crystallographic axial symmetries based upon the combinations in Fig. 13.

Combination of rotation axes, n2



Combination of rotation axes

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The Symmetrical Plane Lattices

Combination of a rotation and a perpendicular



 ⇒ The net motion of the line is therefore equivalent to a rotation about B. Furthermore, since the line is embedded in space, and since the operations $A\alpha$ and t action all spaces,

 \Rightarrow All space must also be rotated about B by this combination of operations.

Point B : lines on the bisector of AA' distance $(AA'/2)cot(\alpha /2)$ from AA'

This can be expressed analytically as

$$\mathbf{A}\boldsymbol{\alpha} \cdot \mathbf{t}_{\perp} = \mathbf{B}\boldsymbol{\alpha}$$

The Symmetrical Plane Lattices

Combination of the rotation axes with a plane lattice :

General principles



1) A rotation axis implies, in general, several related rotations

- When the symmetry axis is n-fold, the smallest rotation is $\alpha = 2\pi/n$
- The rotation axis then implies the rotations α , 2α , ..., $n\alpha$, where $n\alpha = 2\pi$
- Each of these rotations is to be combined with the translation

2) Each rotation must be combined with the various translations of the plane lattice such as t_1 , t_2 , t_1+t_2

A) 2-fold axis : rotation A_{π}



 \therefore B lies in the bisector

(AA'/2) cot (α/2) =0





B) 3-fold axis



It has three non-equivalent 3-fold axis located in the cell at A, B, C.

C) 4-fold axis

The operations of the 4-fold axis are rotations of 1, $\pi/2$, π , $3\pi/2(=-\pi/2)$



Rotation	transl	ations
at A	t ₁	t ₁ +t ₂
1	1	1
π/2	$\pi/2$ at B ₁	$\pi/2$ at C ₁
π	π at B ₂	π at C ₂ (B ₁)
-π/2	$- \pi/2$ at B ₃ (B ₁)	$-\pi/2$ at C ₃ (A')



C) 6-fold axis

When a lattice plane has 6-fold axis, then $t_1 = t_2 = t_1 + t_2 \rightarrow$ Thus, only consider t_1



Lemma : For n>2, the shape of a plane lattice consistent with

pure axial symmetry *n* is also consistent with corresponding

symmetry *nmm* containing reflection planes $m \rightarrow$ Therefore, new lattice-plane mesh types can only be found by causing a general lattice type to be consistent either with symmetry m (or 2mm)







Mesh shape	Symbol	Consistent with plane symmetries
Parallelogram	P	1, 2
120°-rhombus	Н	3, 3m, 6, 6mm
Square	S	4, 4mm
Rectangle	R	
Diamond (rhombus)		m, 2mm



The distribution of rotation axes and mirrors in the five plane lattice types