Homework:

Consider the cubic crystal system. Why is there **no distinct "base-centered cubic" lattice**?

Homework

1.2 By analogy with Table 1.1, determine the number and type of 2D crystal systems via considering their possible minimum symmetry elements and sketching their Bravais lattices.

Table 1.1 Sorting 32 crystallographic point groups into seven crystal systems.

Crystal system	Minimum symmetry	Higher-symmetry point groups
Triclinic	1	$\bar{1}$
Monoclinic	2, *m*	2/m
Orthorhombic	222	*mm*2, *mmm*
Tetragonal	4, $\bar{4}$	4/*m*, 422, 4*mm*, $\bar{4}$ 2*m*, 4/*mmm*
Hexagonal	6, $\bar{6}$	6/*m*, 622, 6*mm*, $\bar{6}$*m*2, 6/*mmm*
Trigonal	3, $\bar{3}$	32, 3*m*, $\bar{3}$*m*
Cubic	23	*m*$\bar{3}$, $\bar{4}$ 3*m*, 432, *m*$\bar{3}$*m*

2-D crystal systems: minimum ↔ maximum point-group symmetry

Crystal system	Unit-cell metric (a,b,γ)	Minimum symmetry (H–M)	Maximum symmetry (H–M)	Intuition for "min → max"
Oblique	$a \neq b,\ \gamma \neq 90^\circ, 60^\circ$	**1** (no symmetry)	**2** (one 180° rotation, C_2)	A generic motif can break C_2; the lattice itself still has a 2-fold (in 2-D this is inversion).
Rectangular	$a \neq b,\ \gamma = 90^\circ$	**m** (one mirror)	**2mm** (C_2 + two perpendicular mirror families)	A motif can keep only one mirror; the lattice has both mirrors and a 2-fold.
Square	$a = b,\ \gamma = 90^\circ$	**4** (four-fold only)	**4mm** (C_4 + mirrors along axes & diagonals)	A motif can remove mirrors but keep C_4; the lattice has the full D_4.
Hexagonal (triangular net)	$a = b,\ \gamma = 60^\circ$	**3** (three-fold only)	**6mm** (C_6 + six mirrors)	A motif can drop to 3-fold; the lattice has the full D_6.

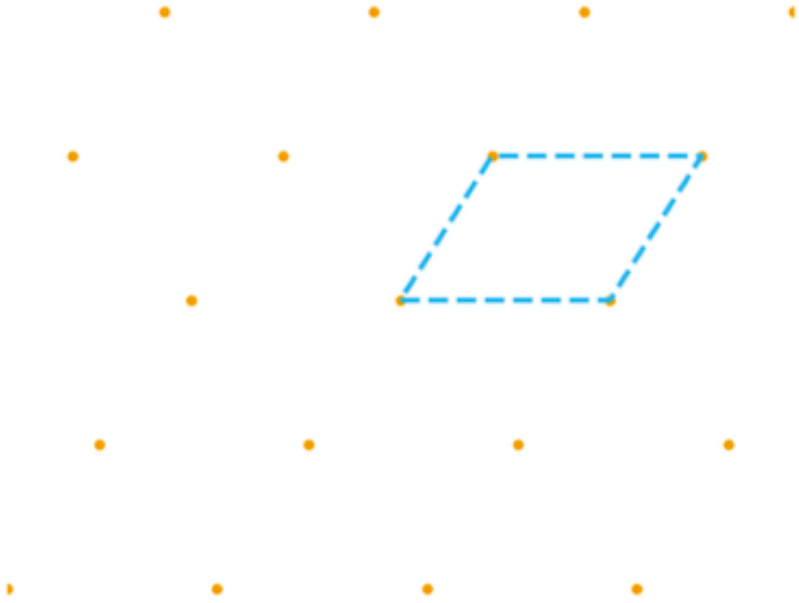
2-D Bravais lattices (5 total)

Bravais lattice	Lattice type	Metric constraints	Notes / equivalences
Oblique (p)	primitive	$a \neq b,\ \gamma \neq 90^\circ, 60^\circ$	General parallelogram.
Rectangular (p)	primitive	$a \neq b,\ \gamma = 90^\circ$	Edges orthogonal, unequal lengths.
Rectangular (c)	**centered**	$a \neq b,\ \gamma = 90^\circ$	Distinct Bravais type. Conventional rectangle has a lattice point at the center; primitive basis can be taken as $\mathbf{u} = \frac{1}{2}(\mathbf{a} + \mathbf{b}), \mathbf{v} = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ (a **rhombus**). Wikipedia
Square (p)	primitive	$a = b,\ \gamma = 90^\circ$	Any "centered square" reduces to a primitive square via a 45° rotation and rescale (not a new Bravais type).
Hexagonal / Triangular (p)	primitive	$a = b,\ \gamma = 60^\circ$	Often called "triangular" in 2-D. Any centering is equivalent to primitive.

Aspect	Crystal system	Bravais lattice
What is classified?	Sets of **point groups** (rotations/mirrors about a fixed point)	Sets of **vector lattices** (translations) distinguished up to centering
Includes translations?	**No**	**Yes** (pure translations only; point symmetry comes from the lattice metric)
What it fixes	Cell **metric**/shape constraints (e.g., $a = b$, $\gamma = 90^\circ$ for square)	Metric **and** whether a **distinct centering** exists (e.g., primitive vs centered)
2-D inventory	**4 systems:** oblique, rectangular, square, hexagonal	**5 Bravais types:** p-oblique, p-rectangular, **c-rectangular**, p-square, p-hexagonal
3-D inventory	**7 systems:** triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, cubic	**14 Bravais types** (e.g., cubic-P, cubic-I, cubic-F; orthorhombic-P/C/I/F; etc.)
Example mapping	"Square system" (requires $a = b,\ \gamma = 90^\circ$)	Within square: only **p-square** (any 'centered square' reduces to p-square). Rectangular admits **p** and **c**.

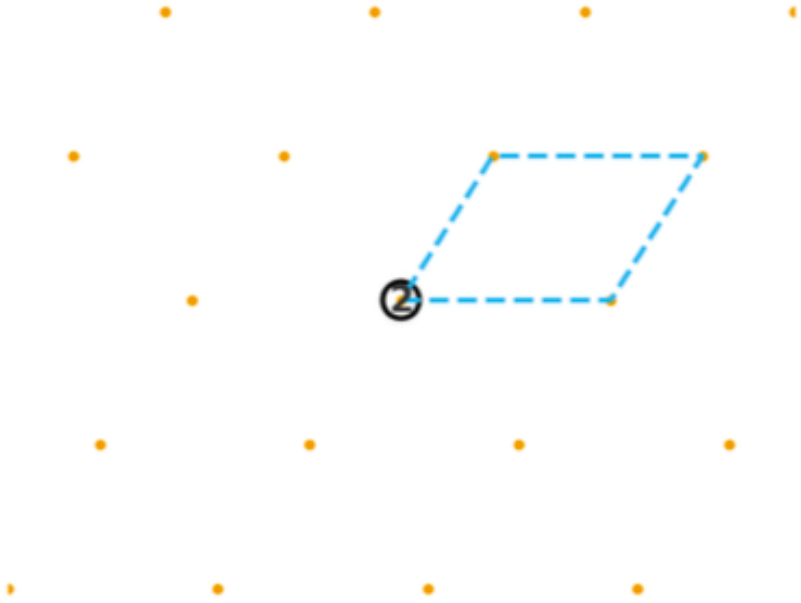
Oblique — min: 1

Oblique — minimum symmetry: 1



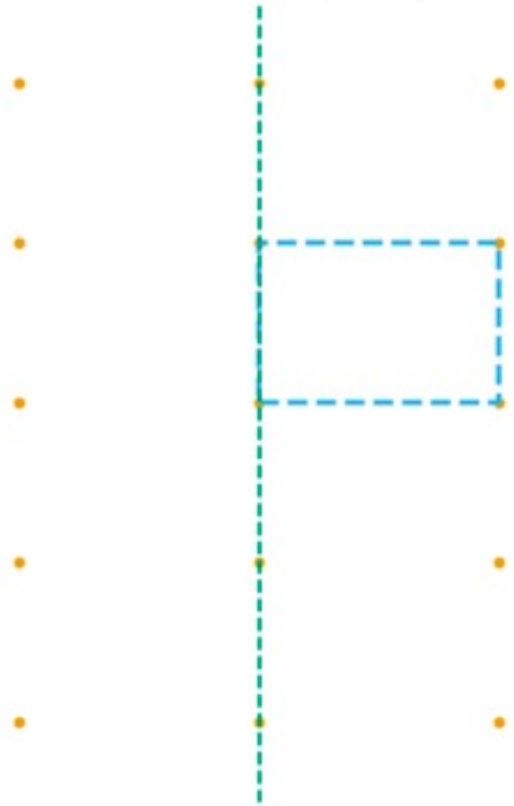
Oblique — max: 2

Oblique — maximum symmetry: 2



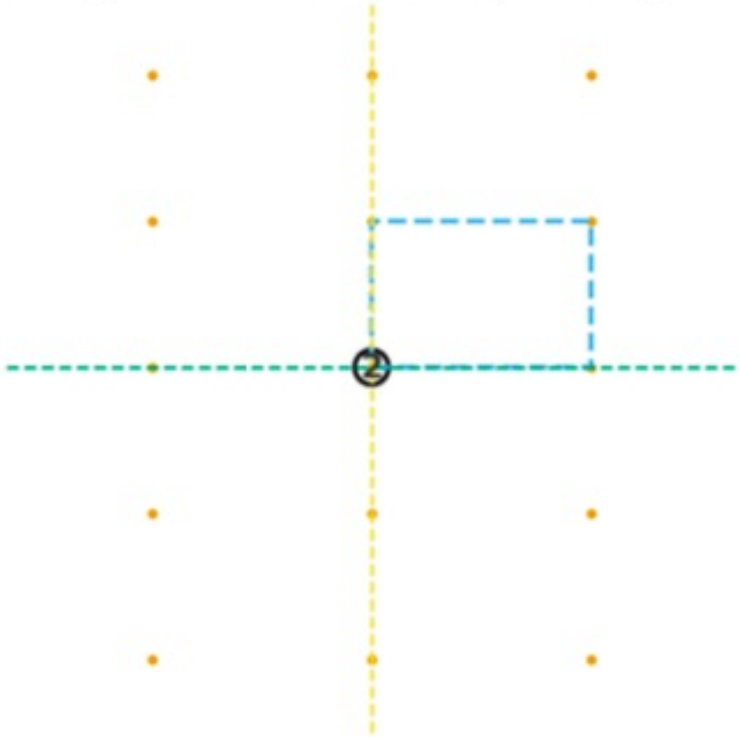
Rectangular — min: m

Rectangular — minimum symmetry: m



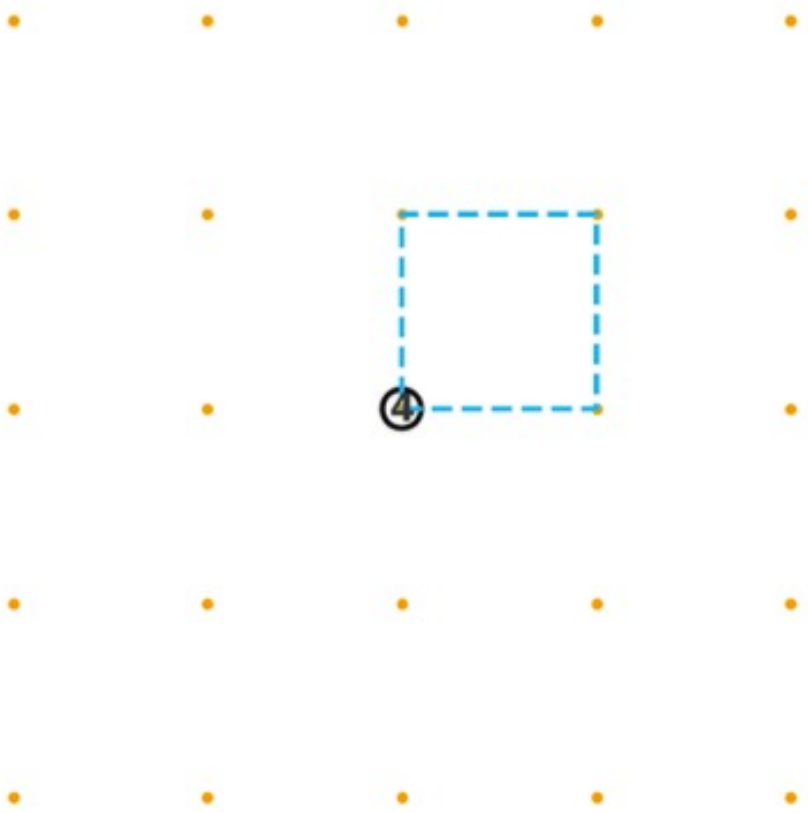
Rectangular — max: 2mm

Rectangular — maximum symmetry: 2mm



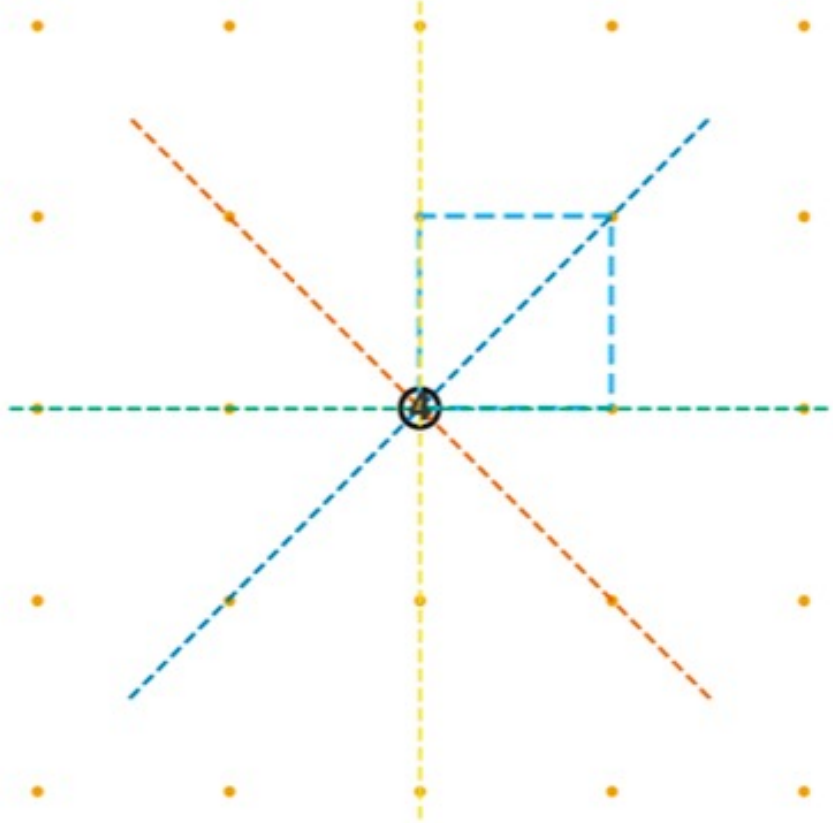
Square — min: 4

Square — minimum symmetry: 4



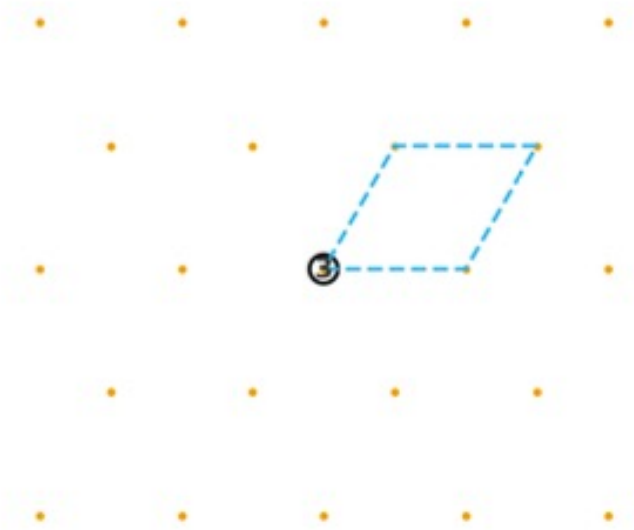
Square — max: 4mm

Square — maximum symmetry: 4mm



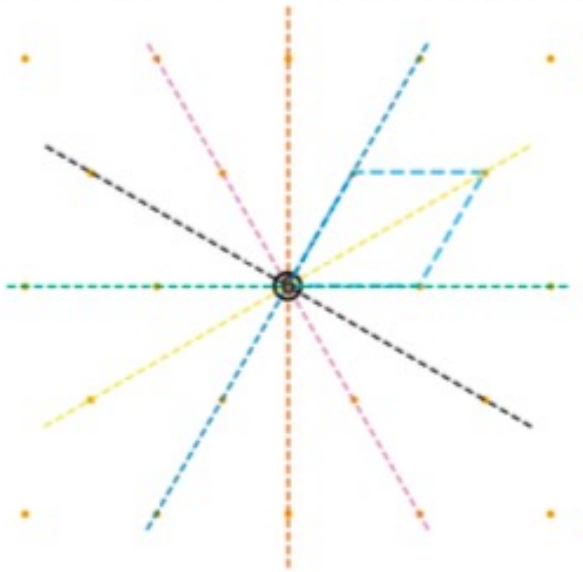
Hexagonal — min: 3

Hexagonal (triangular net) — minimum symmetry: 3

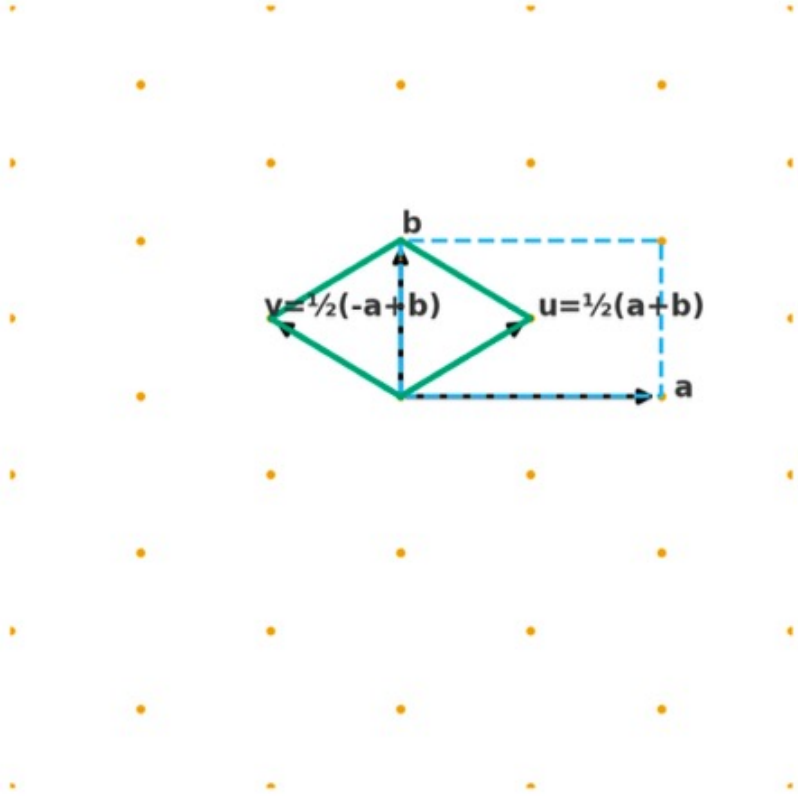


Hexagonal — max: 6mm

Hexagonal (triangular net) — maximum symmetry: 6mm



Bravais: Rectangular (centered) — dashed: conventional; solid: primitive rhombus



Learning Objectives

- Define and describe the basic crystallographic point-symmetry elements (identity, inversion, mirror, rotation, rotoinversion).
- Distinguish between point groups (fixed point symmetry only) and space groups (point symmetry plus translation).
- Recognize and interpret non-symmorphic symmetry elements (glide planes and screw axes).
- Understand why only 2-, 3-, 4-, and 6-fold rotations are compatible with a lattice.
- Relate sets of symmetry elements to crystal systems, with the idea that these are organized into the 32 crystallographic point groups.

What is a Symmetry Operation?

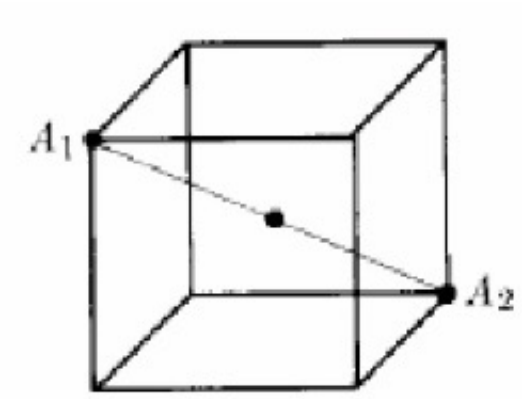
A **symmetry operation** is any transformation (rotation, reflection, inversion, translation, etc.) that maps a structure **onto itself** — i.e. after applying it, the object is indistinguishable from where it started.

Symmetry is a way crystallographers classify different types of crystals.

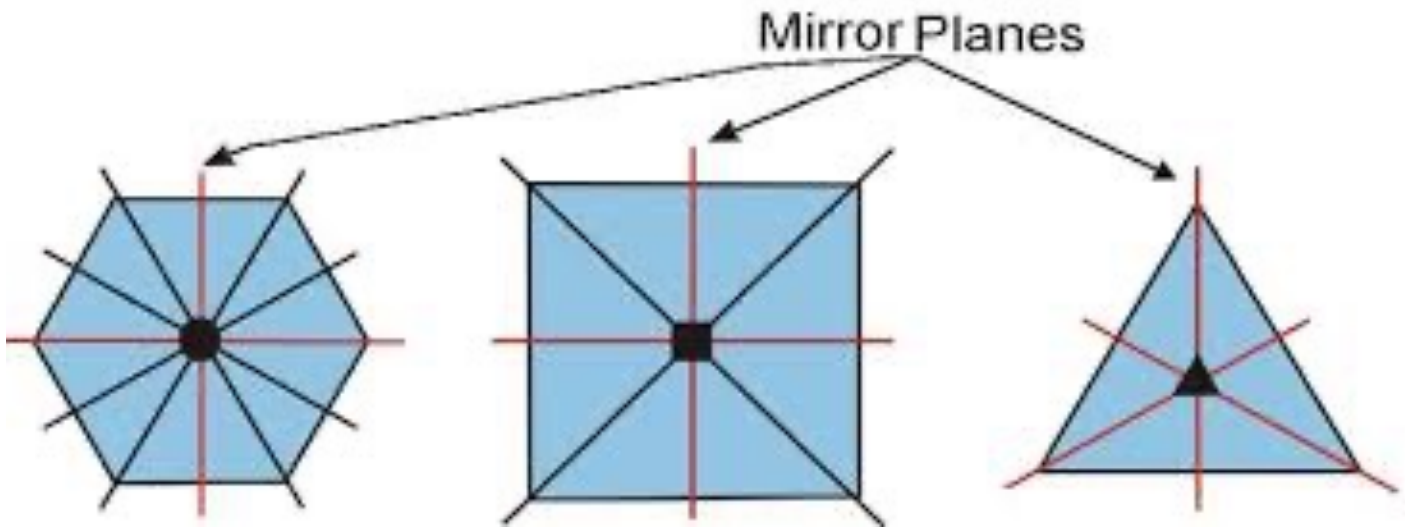
Point Symmetry Elements

Point Symmetry Element	Symmetry Operation
1. Identity (1)	Nothing changes
2. Inversion center ($\bar{1}$)	Inversion through a point
3. Mirror plane (*m*)	Reflect through the plane
4. Proper rotation axis (N)	Rotate by 360/N degrees about the axis
5. Rotoinversion axis ($\bar{N}$)	Rotate by 360/N degrees about the axis, followed by inversion operation

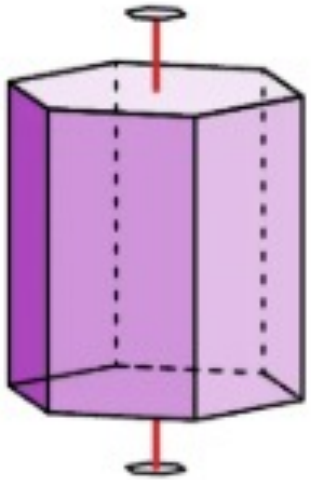
Inversion Center



- Inversion through a point, called the center of symmetry


Mirror Planes

sixfold axis of rotation

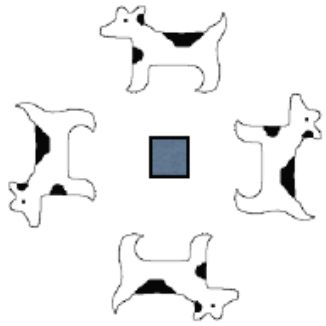


When rotated about its axis, the crystal repeats itself every 60° (six times in a 360° rotation).

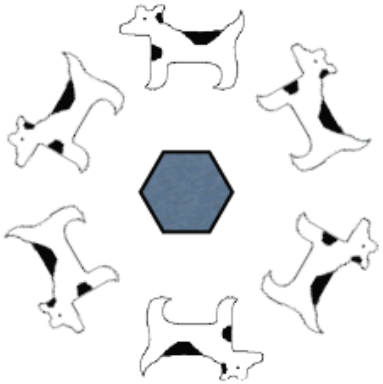
An n fold rotational symmetry operation rotates an object by 360°/n. Only n = 1, 2, 3, 4, and 6 are permitted in a periodic lattice

2 fold
'Diad'

3 fold
'Triad'

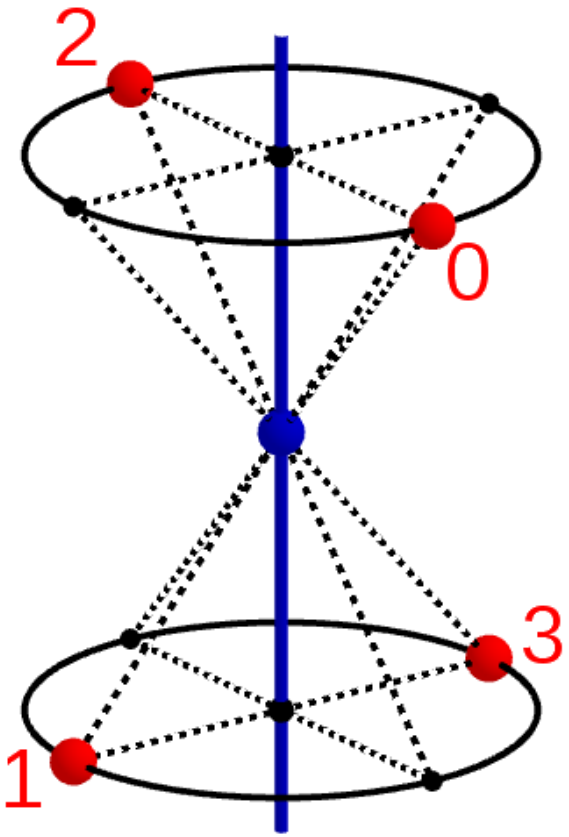


4 fold
'Tetrad'



6 fold
'Hexad'

RotoInversion



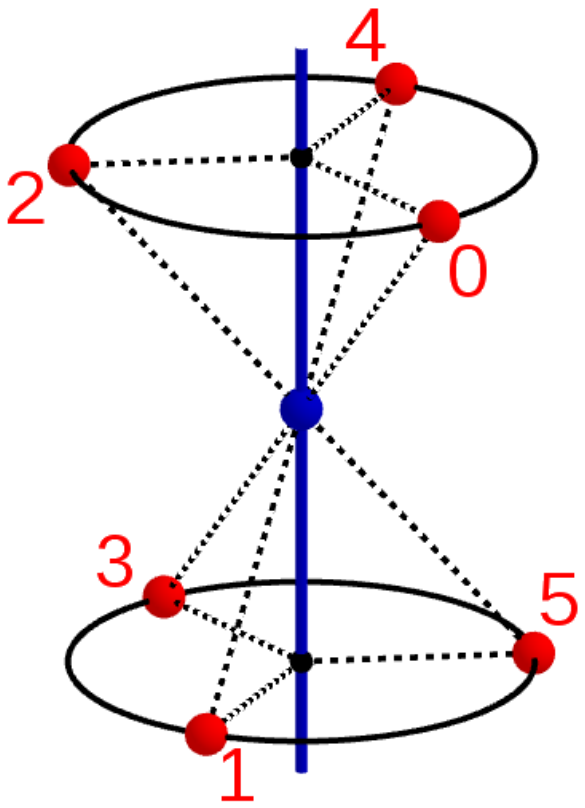


Table 1.28 ***Point symmetry elements***

Symmetry element	Written symbol	Graphical symbol
Rotation axes	1	None
	2	
	3	
	4	
	6	
Inversion axes	$\bar{1}$	None[a]
	$\bar{2}(\equiv m)$	[b]
	$\bar{3}(\equiv 3+\bar{1})$	
	$\bar{4}$	
	$\bar{6}(=3/m)$	
Mirror plane	m	

[a] The inversion axis, $\bar{1}$, equivalent to a centre of symmetry, is represented as a small open circle, o, in space groups, but does not have a formal graphical representation in point groups, even though it is present in many point groups.

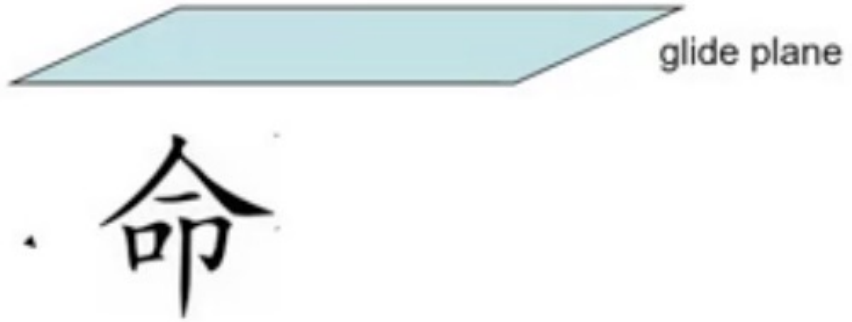
[b] The inversion axis, $\bar{2}$ does not have a separate graphical symbol other than that of the mirror plane equivalent to it.

From West, Solid State Chemistry and its Applications

Point & Composite Symmetry Elements

Point Symmetry Element	Symmetry Operation
1. Identity (1)	Nothing changes
2. Inversion center ($\bar{1}$)	Inversion through a point
3. Mirror plane (*m*)	Reflect through the plane
4. Proper rotation axis (N)	Rotate by 360/N degrees about the axis
5. Rotoinversion axis ($\bar{N}$)	Rotate by 360/N degrees about the axis, followed by inversion operation
6. Glide plane (*a*, *b*, *c*, *n*, *d*)	Reflect through a plane, then translate parallel to the plane
7. Screw axis (N_M)	Rotate by 360/N degrees about the axis, followed by a translation by M/N of the unit cell parallel to the axis

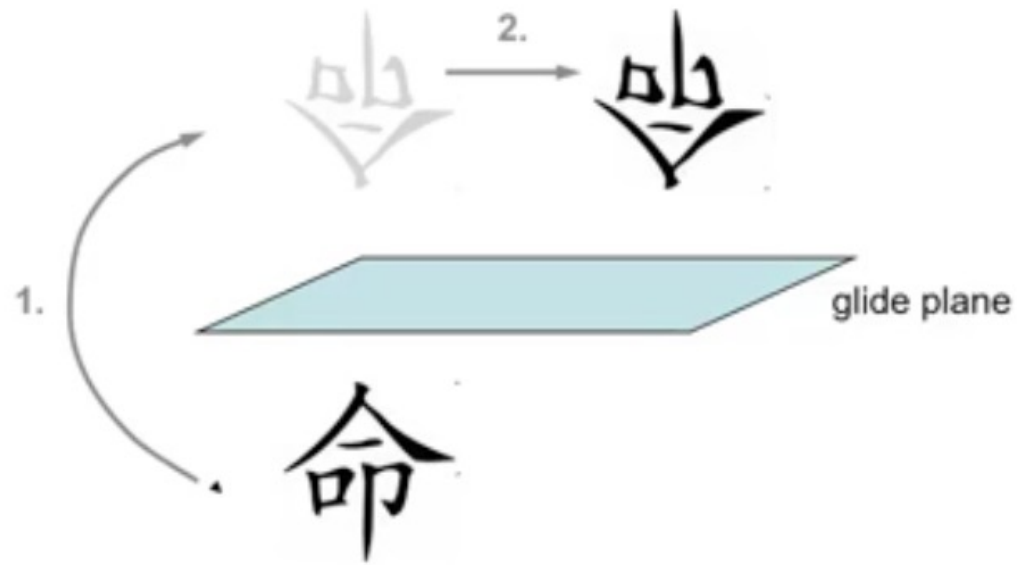
Glide Planes



1. Reflect through the glide plane
(just as with a mirror plane)

2. Translate parallel to the glide plane

Glide Planes



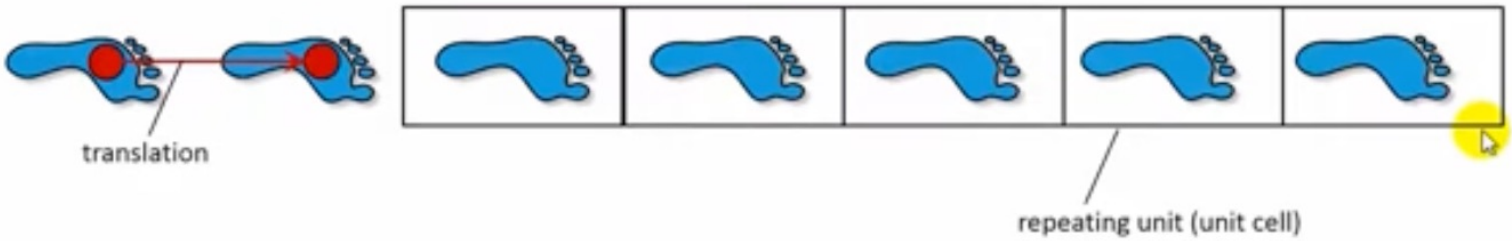
1. Reflect through the glide plane
(just as with a mirror plane)

2. Translate parallel to the glide plane

Translational Symmetry

- There are three symmetry elements, which have a translational component

    1. Translation (in units of whole unit cells along the lattice vectors)



Translational Symmetry

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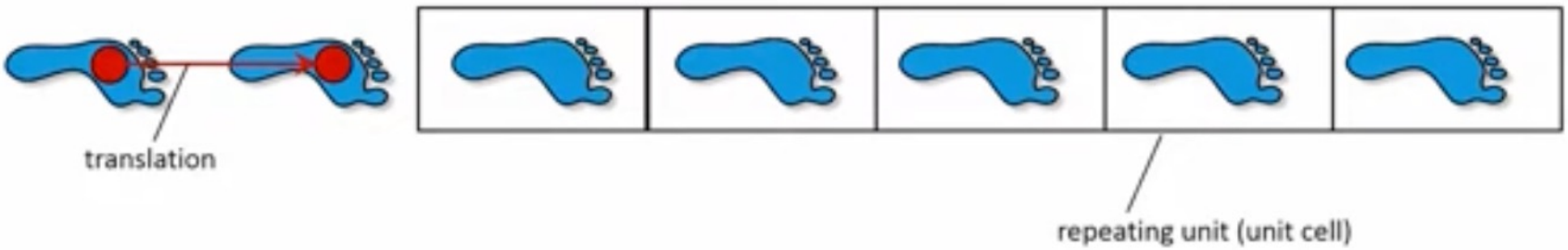
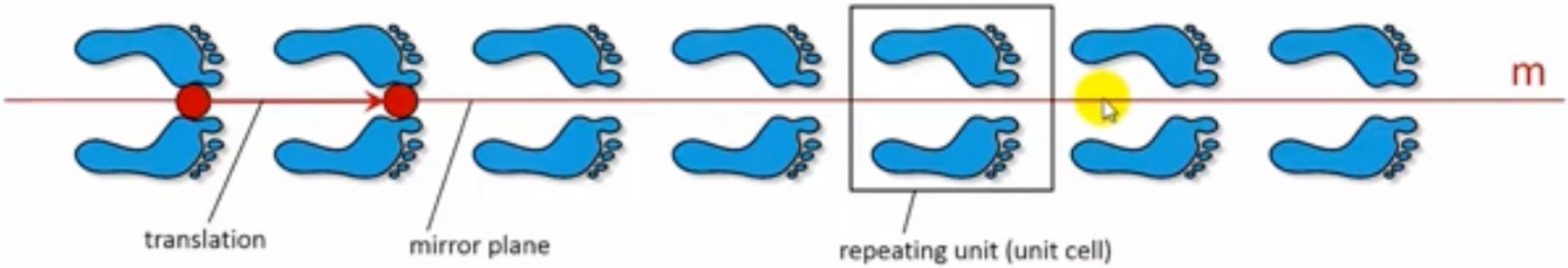
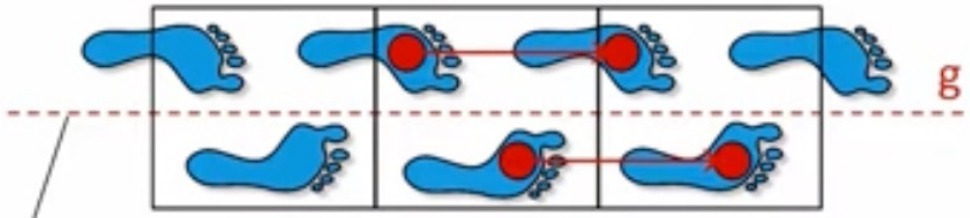




Glide planes/lines

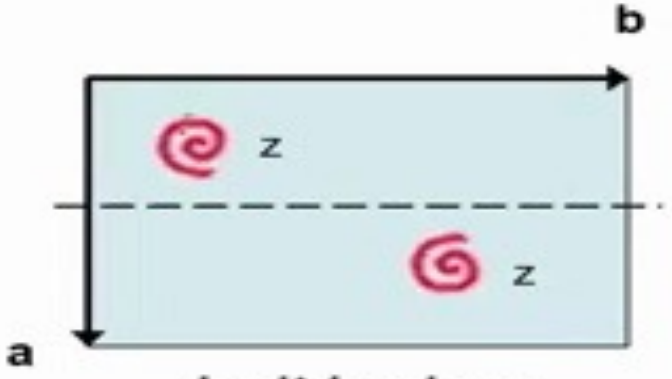


glide line

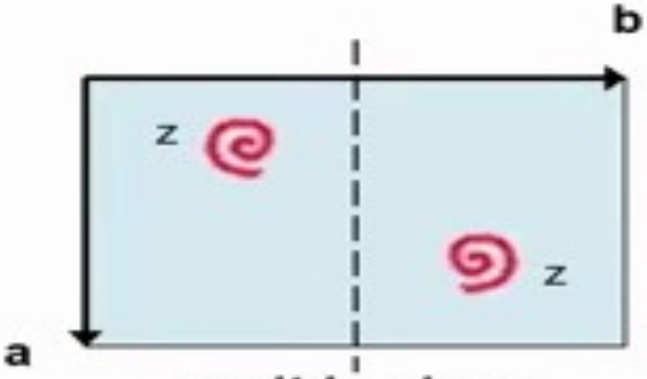
glide reflection →

(a) reflection at a plane / line
(b) translation (usually by $^1/_2$ of the unit cell)

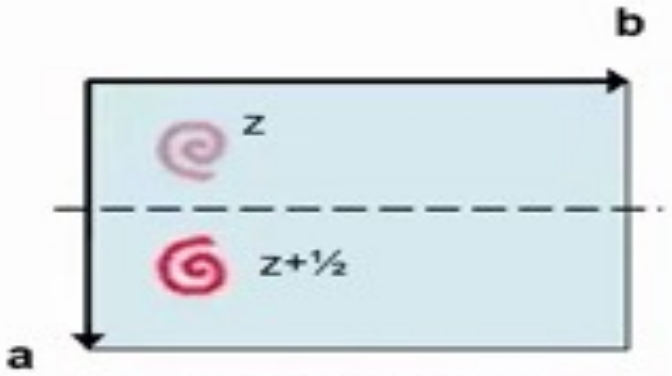
Types of Glide Planes



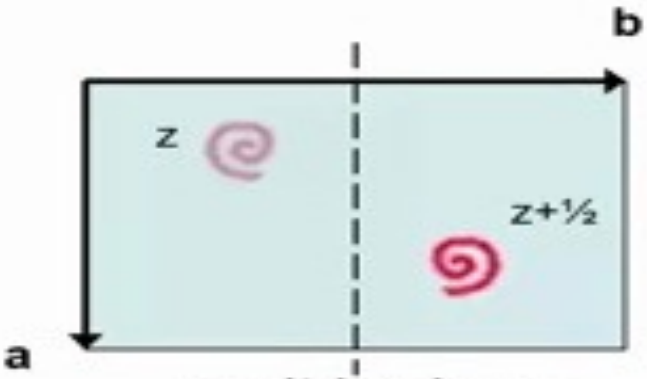
b glide plane
translate by ½ **b**



a glide plane
translate by ½ **a**



c glide plane
translate by ½ **c**



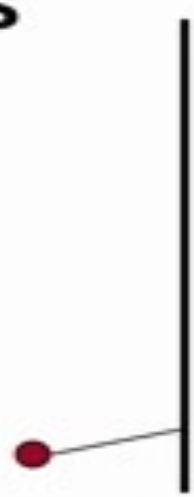
n glide plane
translate by ½ **a** + ½ **c**

Types of Glide Planes

Herman-Mauguin Symbol	Plane ⊥ to which axis	Translation vector
Axial Glides		
a	b or c	½ **a**
b	a or c	½ **b**
c	a or b	½ **c**
Diagonal glides, *n*	a	½ **b** + ½ **c**
	b	½ **a** + ½ **c**
	c	½ **a** + ½ **b**
Diamond glides, *d*	a	¼ **b** + ¼ **c**
	b	¼ **a** + ¼ **c**
	c	¼ **a** + ¼ **b**

N_M Screw Axes

2_1 screw axis
Rotate by 180°
Translate by ½ **c**

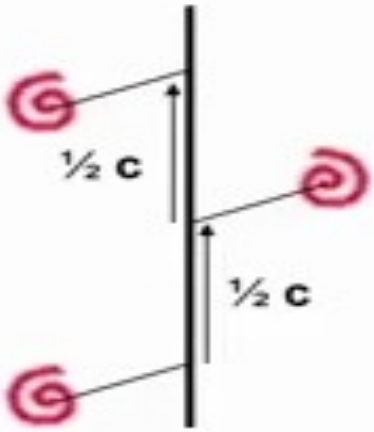


4_1 screw axis
Rotate by 90°
Translate by ¼ **c**

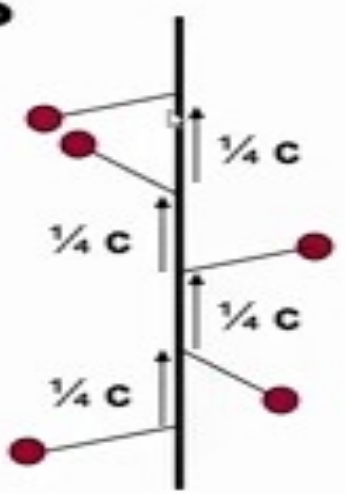
1. Rotate by 360/N (just as with a N-fold proper rotation axis)

2. Translate by *M*/N of a unit cell vector parallel to the screw axis

N_M Screw Axes



2_1 screw axis
Rotate by 180°
Translate by ½ **c**



4_1 screw axis
Rotate by 90°
Translate by ¼ **c**

1. Rotate by 360/N (just as with a N-fold proper rotation axis)

2. Translate by *M*/N of a unit cell vector parallel to the screw axis

Point Groups

A point group is a set of operations (point symmetry elements) that fulfil the mathematical requirements of being a group and act on an isolated object.

A group must

- have a closure (combination of two elements yields an element of the group),
- obey the associative law (the result of combination of the elements is independent of the order they are applied), have an
- have an identity (an element that converts other elements into themselves),
- have an inversion (every element has an inverse element; when combined together, they yield the identity element)

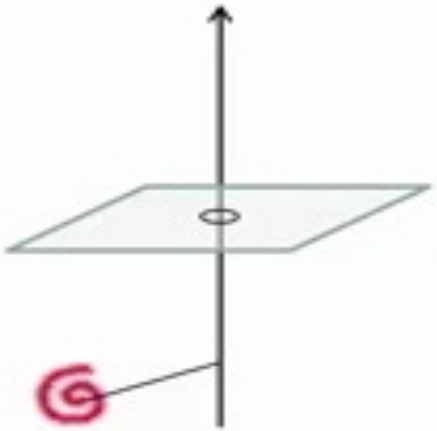
Question

Let's take a twofold rotation axis. And let's have a mirror plane perpendicular to it.

Is that a valid point group, just those two symmetry operations?

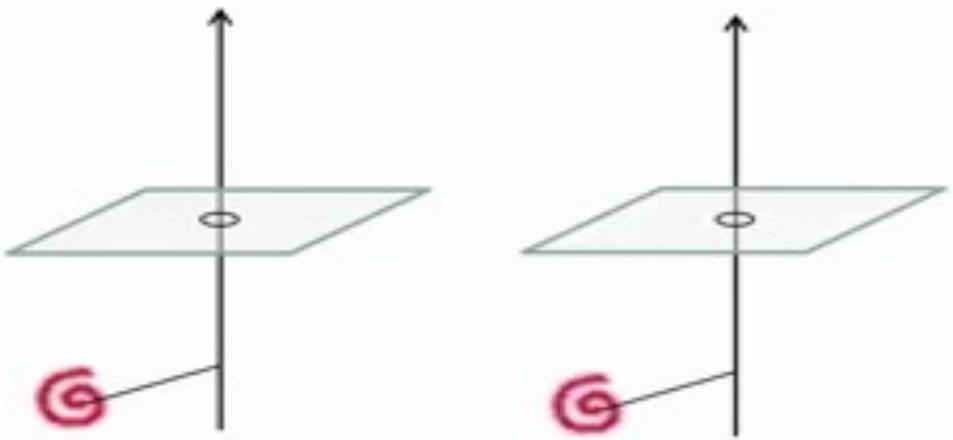
If not, what other symmetry operations do we need to add to those two operations or elements to get a valid point group?

Point group 2/m (C_{2h})



identity

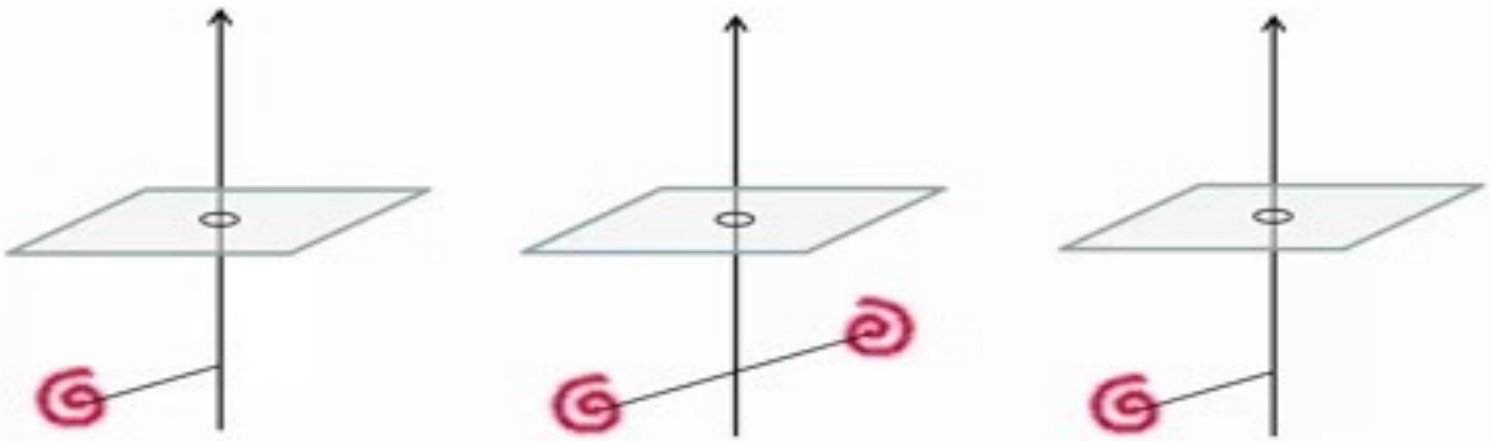
Point group 2/m (C_{2h})



identity

2-fold
rotation

Point group 2/m (C_{2h})

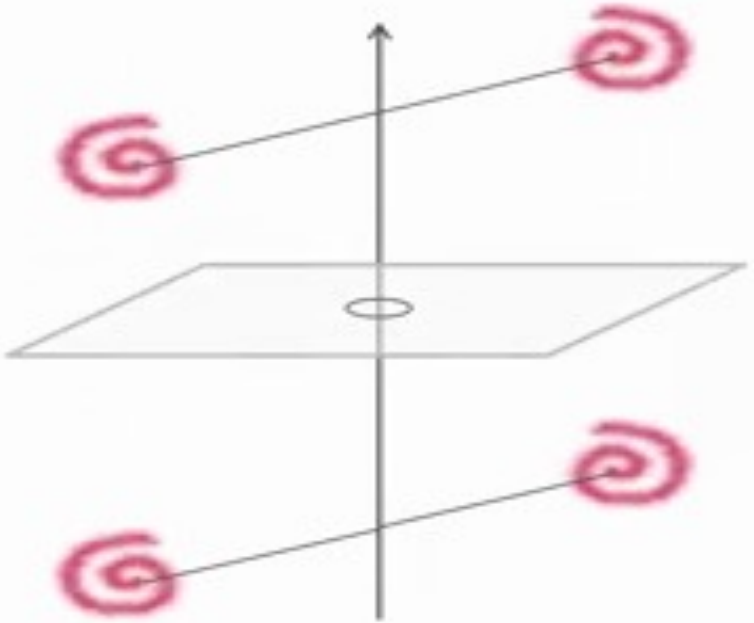


identity

2-fold rotation

mirror plane

Point group 2/m (C_{2h})



32 Crystallographic Point Groups

Crystal System	Unit Cell	Required symmetry	Point groups
Cubic	Cubic	3-fold axes along body diagonal	$23, m\bar{3}, \bar{4}3m, 432, m\bar{3}m$
Tetragonal	Tetragonal	4-fold axis	$4, \bar{4}, 4/m, 422, 4mm, \bar{4}m2, 4/mmm$
Hexagonal	Hexagonal	6-fold axis	$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/mmm$
Trigonal	Hexagonal or Rhombohedral	3-fold axis	$3, \bar{3}, 32, 3m, \bar{3}m$
Orthorhombic	Orthorhombic	Three mutually perpendicular 2-fold axes or mirror planes	$222, 2mm, mmm$
Monoclinic	Monoclinic	2-fold axis or mirror plane	$2, m, 2/m$
Triclinic	Triclinic	none	$1, \bar{1}$

Who Cares about Point Groups?

- This classification gives a “shorthand” for the full set of symmetries — instead of listing all operations one by one, you just say “C_2v” or “$m\bar{3}m$” and an expert immediately knows the symmetries present.
- Many physical properties (optical, electrical, mechanical) depend directly on the symmetry of the crystal:
- **Piezoelectricity** only occurs in non-centrosymmetric point groups.
- **Ferroelectricity** only occurs in certain polar point groups.
- **Optical anisotropy (birefringence)** depends on whether the point group has rotational symmetry axes that constrain refractive indices.
- By knowing the point group, you can immediately rule in or rule out whole classes of properties.

Schoenflies & Hermann Mauguin

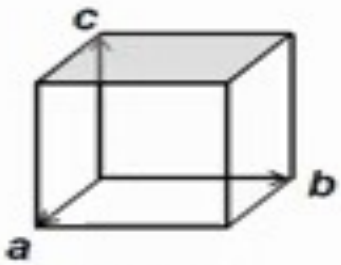
Crystal System	Unit Cell	Hermann-Mauguin Point groups	Schoenflies Point groups
Cubic	Cubic	$23, m\bar{3}, \bar{4}3m, 432, m\bar{3}m$	T, T_h, T_d, O O_h
Tetragonal	Tetragonal	$4, \bar{4}, 4/m, 422, 4mm, \bar{4}m2, 4/mmm$	C_4, S_4, C_{4h}, D_4 C_{4v}, D_{2d}, D_{4h}
Hexagonal	Hexagonal	$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/mmm$	C_6, C_{3h}, C_{6h}, D_6 C_{6v}, D_{3h}, D_{6h}
Trigonal	Hexagonal or Rhombohedral	$3, \bar{3}, 32, 3m, \bar{3}m$	$C_3, C_{3i}, D_3, C_{3v}, D_{3d}$
Orthorhombic	Orthorhombic	$222, 2mm, mmm$	D_2, C_{2v}, D_{2h}
Monoclinic	Monoclinic	$2, m, 2/m$	C_2, C_s, C_{2h}
Triclinic	Triclinic	$1, \bar{1}$	C_1, C_i

Homework

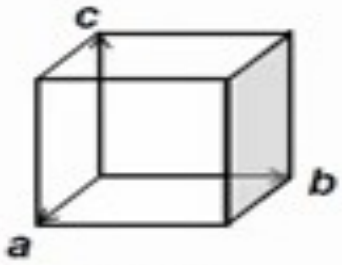
- List the five fundamental point-symmetry elements and briefly describe what each does.

- Why are only 2-, 3-, 4-, and 6-fold rotations allowed in crystals?

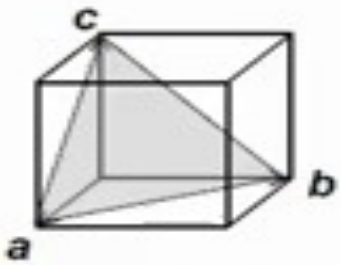
Directions in Crystals



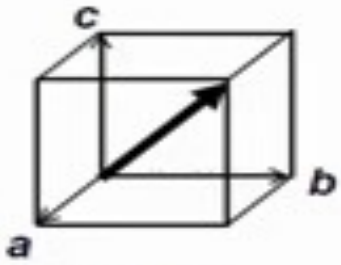
a single
(001) plane



a single
(010) plane



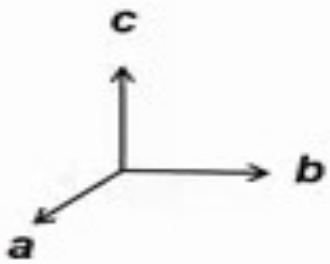
a single
(111) plane

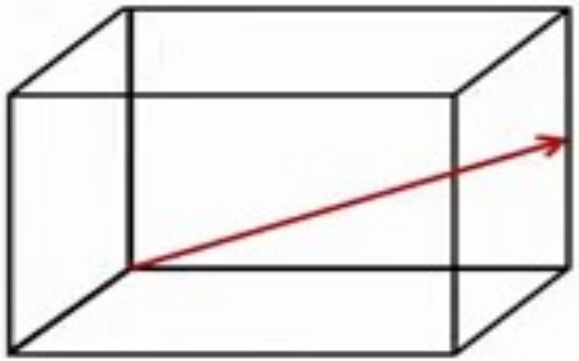


a [111]
direction

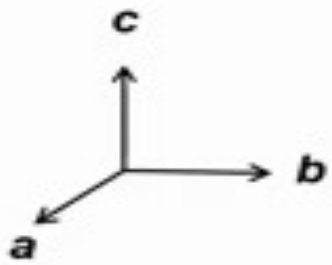
Directions in a crystalline lattice are represented as [*uvw*], where *u*, *v and w* are the fractional coordinates of any point that a line extending from the origin intersects with. By convention we normally use the smallest set of integers for *uvw*. [121] = [½ 1 ½] = [242]

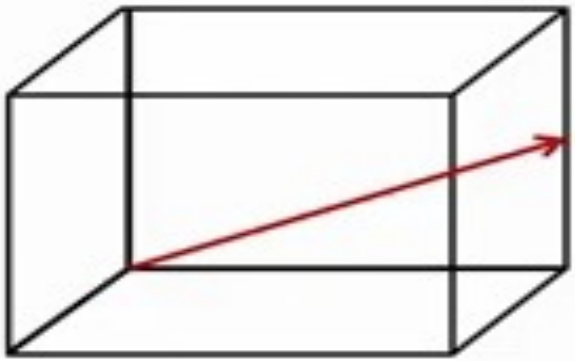
What direction is shown below?



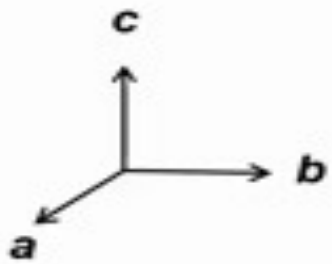


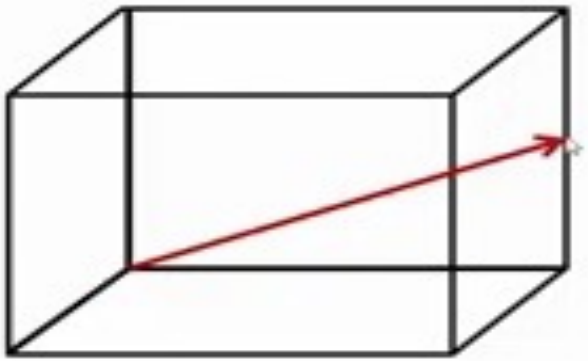
What direction is shown below?





What direction is shown below?



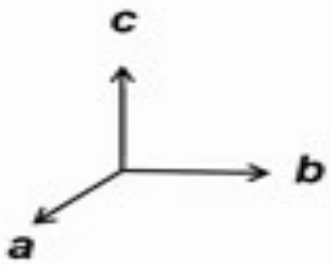


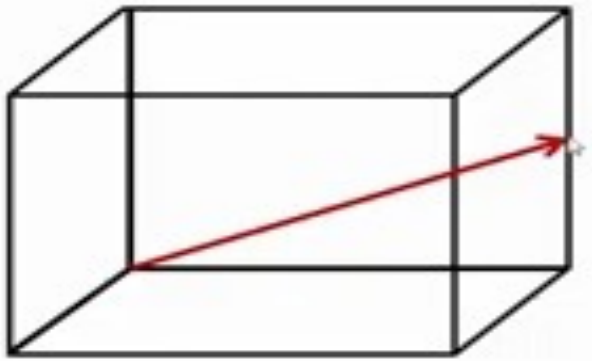
Coordinates where it crosses
the unit cell boundary

a = 0
b = 1
c = ½

→ ***R*** = ***b*** + ½***c***

What direction is shown below?



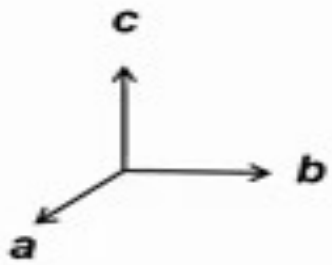


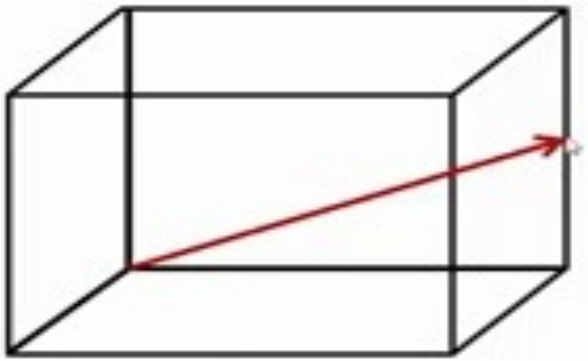
Coordinates where it crosses
the unit cell boundary

a = 0
b = 1
c = ½

→ ***R*** = ***b*** + ½***c***

What direction is shown below?



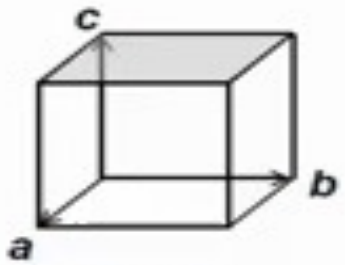


Coordinates where it crosses
the unit cell boundary

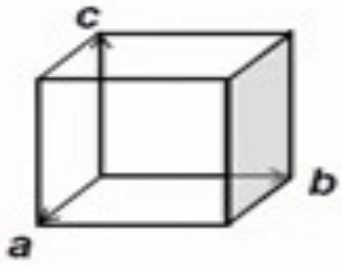
a = 0
b = 1
c = ½

→ ***R*** = ***b*** + ½***c*** → [021]

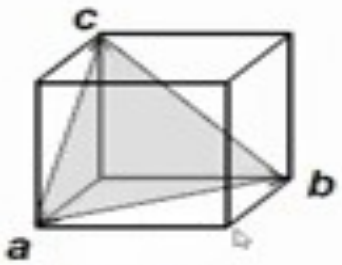
Miller Indices of Equivalent Planes



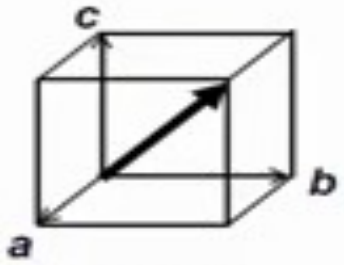
a single
(001) plane



a single
(010) plane



a single
(111) plane

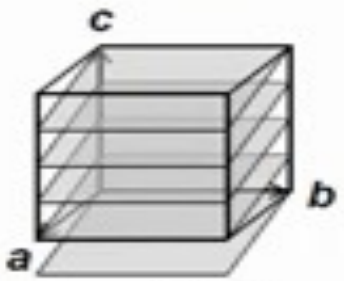


a [111]
direction

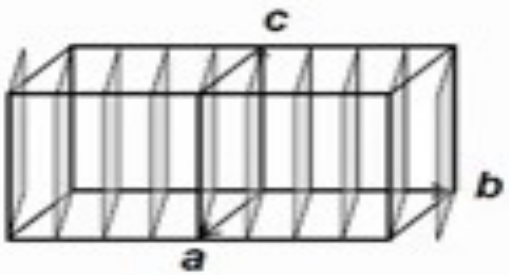
Sets of equidistant parallel planes in a crystalline lattice are represented as (*hkl*). These values are often called Miller Indices. To determine the values of *h*, *k* and *l* we look at the plane that is next to the plane that goes through the origin and determine its intercepts with the lattice vectors ***a***, ***b*** and ***c***.

h = to 1/(***a*** intercept)
k = to 1/(***b*** intercept)
l = to 1/(***c*** intercept)

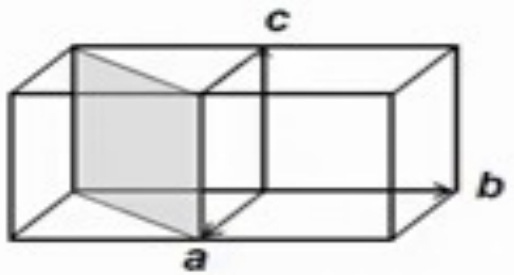
Equivalent Planes in Crystals



several (104)
equidistant planes

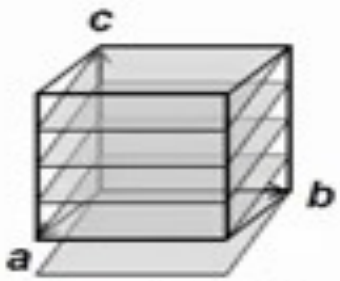


several $(1\bar{4}0)$
equidistant planes



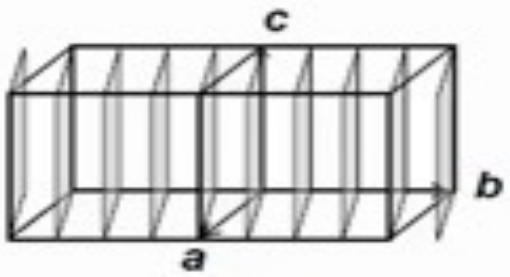
a single
$(1\bar{1}0)$ plane

Equivalent Planes in Crystals



several (104)
equidistant planes

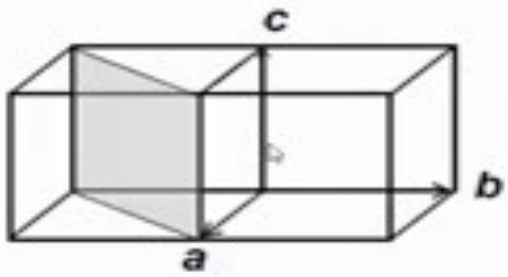
Intercepts
a at 1
b no intercept
c at ¼



several $(1\bar{4}0)$
equidistant planes

Intercepts
a at 1
b at −¼
c no intercept

Equivalently we
could use $(\bar{1}40)$

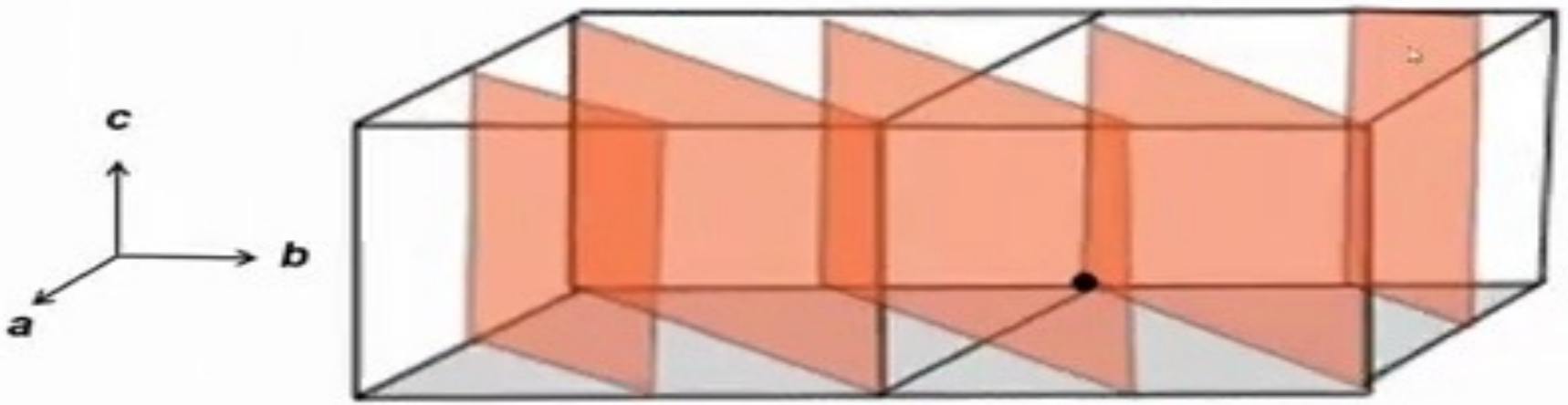


a single
$(1\bar{1}0)$ plane

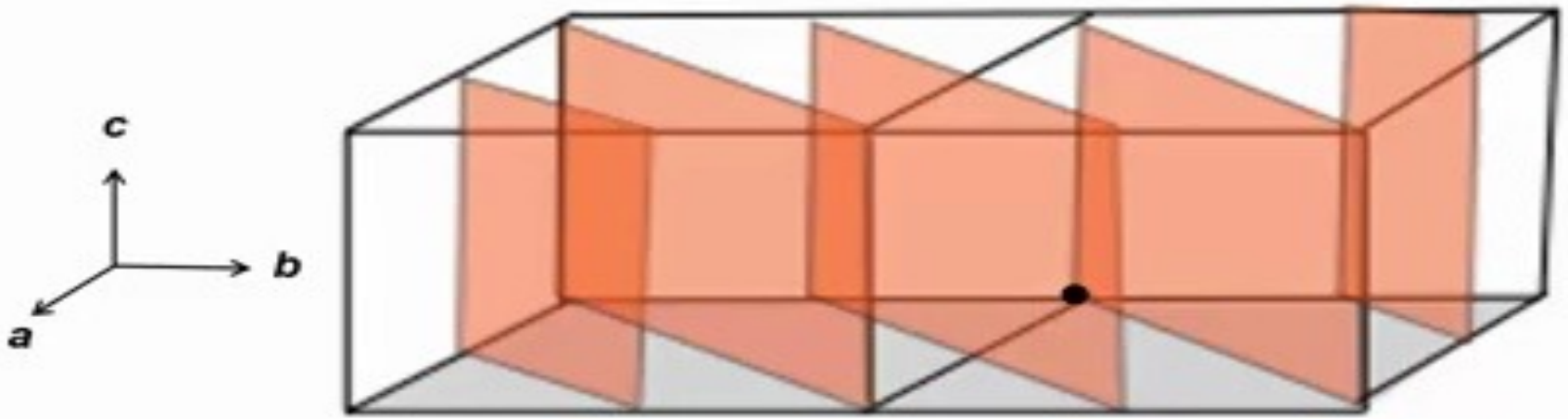
Intercepts
a at 1
b at −1
c no intercept

Equivalently we
could use $(\bar{1}10)$

What are the Miller Indices for the set of planes shown below?



What are the Miller Indices for the set of planes shown below?



Intercepts
a at ½
b at – ½
c no intercept

→ $(2\bar{2}0)$

Symmetrically Equivalent Directions and Lattice Planes

In certain lattices different directions can be equivalent due to symmetry. For example, in a cubic crystal the [100], [010], [001], $[\bar{1}00]$, $[0\bar{1}0]$ and $[00\bar{1}]$ directions are all symmetrically equivalent. We refer to this set of equivalent directions with angled brackets $\langle 100 \rangle$.

Similarly, a collection of equivalent lattice planes is denoted with curly brackets. For example, $\{100\}$ represents the (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$ and $(00\bar{1})$ lattice planes in a cubic crystal.

Homework Question

1.1 Write down the $\langle 111 \rangle$ set of symmetry-equivalent directions in a cubic lattice.