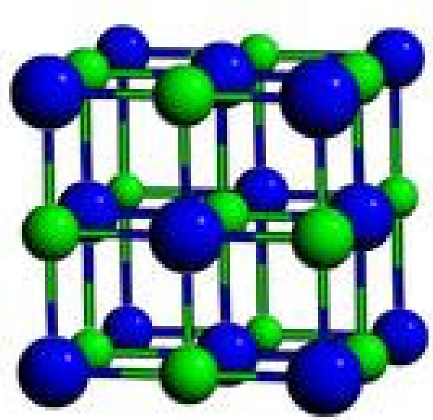
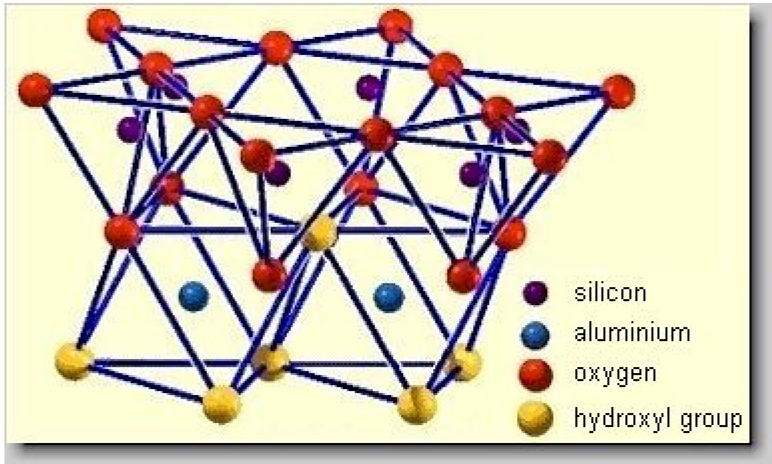
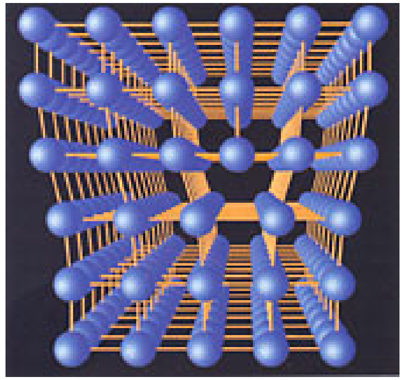
Chapter 7 14 Bravais Lattice







Reading Assignment:

1. W. B-Ott, Crystallography-chapter 6

http://www.greenfacts.org/glossary/abc/crystal-lattice.htm

Contents

14 Bravais Lattice

- general space lattice- inversion center

  special space lattice- rotation axis and mirror plane

  - restriction on the cell parameters

    ex) 4_z-fold rotation axis- a=b, $\gamma=90^o$

  - simplifications in the crystal morphology

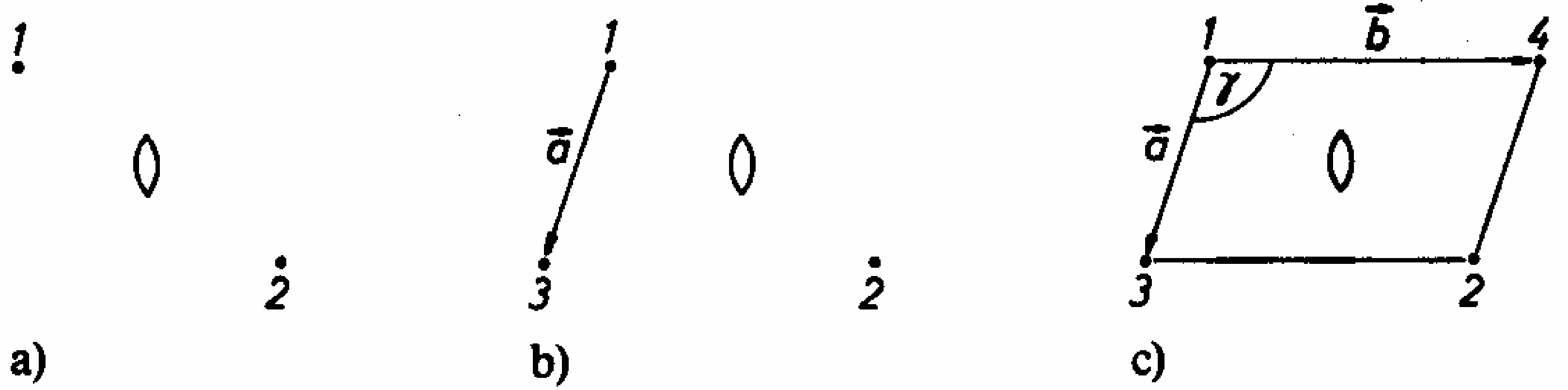
    and in the physical properties

Plane Lattice

-general (oblique) lattice

2 fold axis: 1 → 2
lattice translation $\vec{a}$: 1 → 3
2 fold axis: 3 → 4

oblique parallelogram $a_o \neq b_o \quad \gamma \neq 90^o$



Plane Lattice

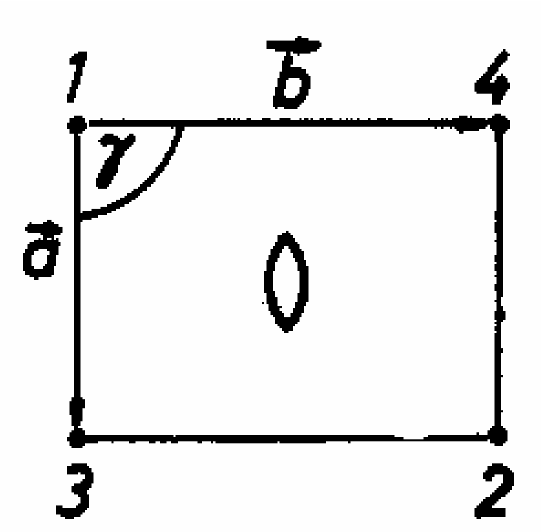
- special lattice

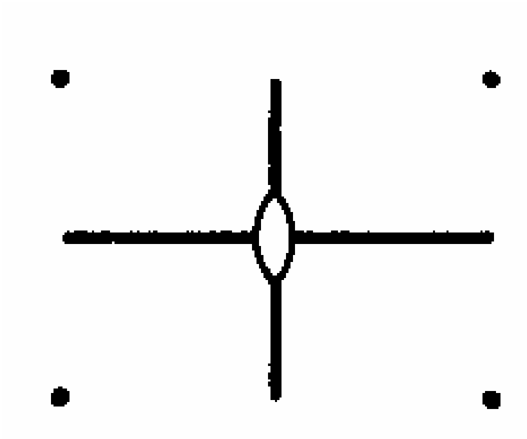
a) $\angle 132 = 90^{\circ}$

$a_o \neq b_o \quad \gamma = 90^{\circ}$

rectangular unit mesh

two perpendicular mirror plane





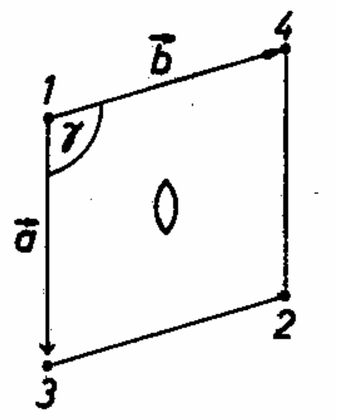
b) $\overline{13} = \overline{23}$

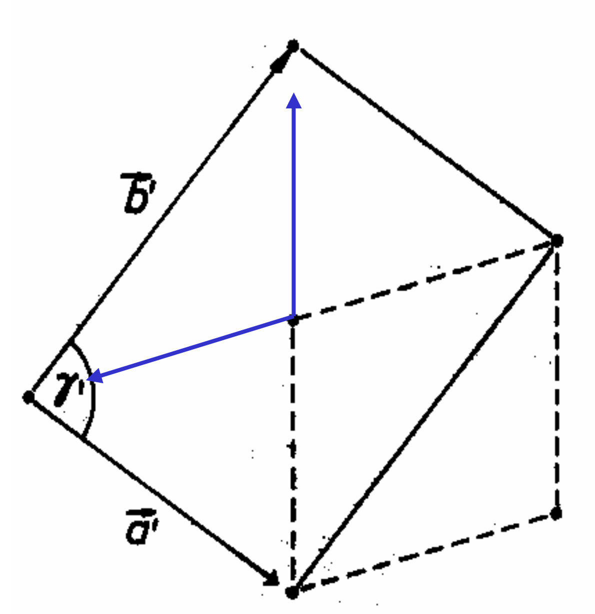
$\angle 132 \neq 60^o, 90^o \text{ or } 120^o$

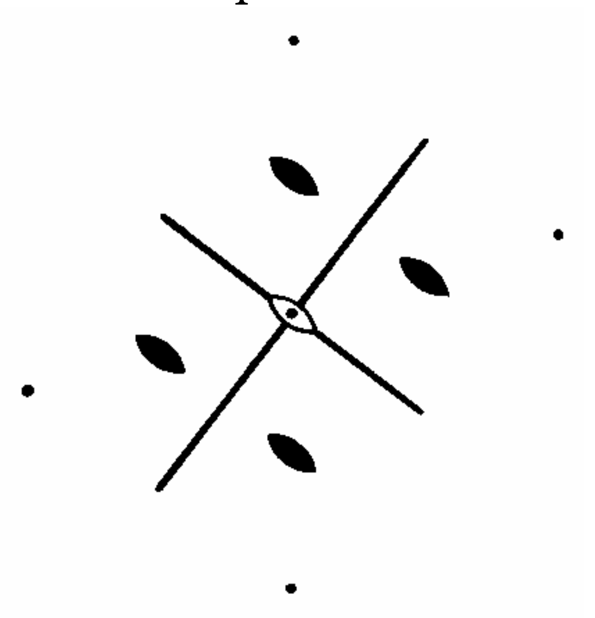
extension of the edges $\overline{13}$ and $\overline{14}$

$a_o \neq b_o \quad \gamma = 90^o$ centered rectangular

2-fold axis, mirror plane







Plane Lattice

c) $\overline{13} = \overline{23}$

$\angle 132 = 90^o$

$a_o = b_o \quad \gamma = 90^o$

square mesh

4-fold axis, mirror plane

d) $\overline{13} = \overline{23}$

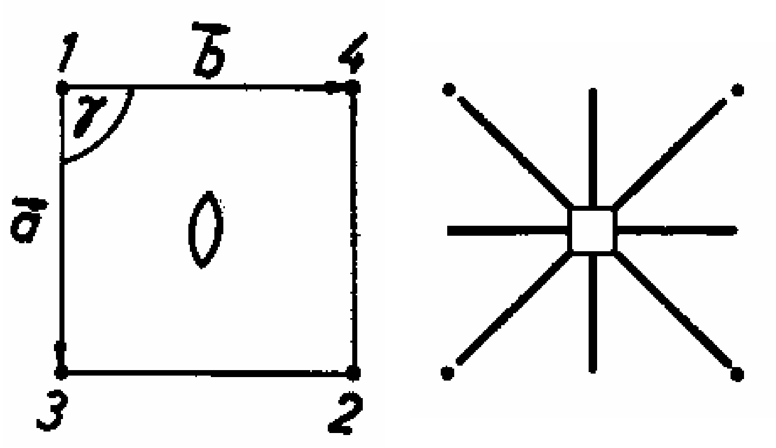
$\angle 132 = 120^o$

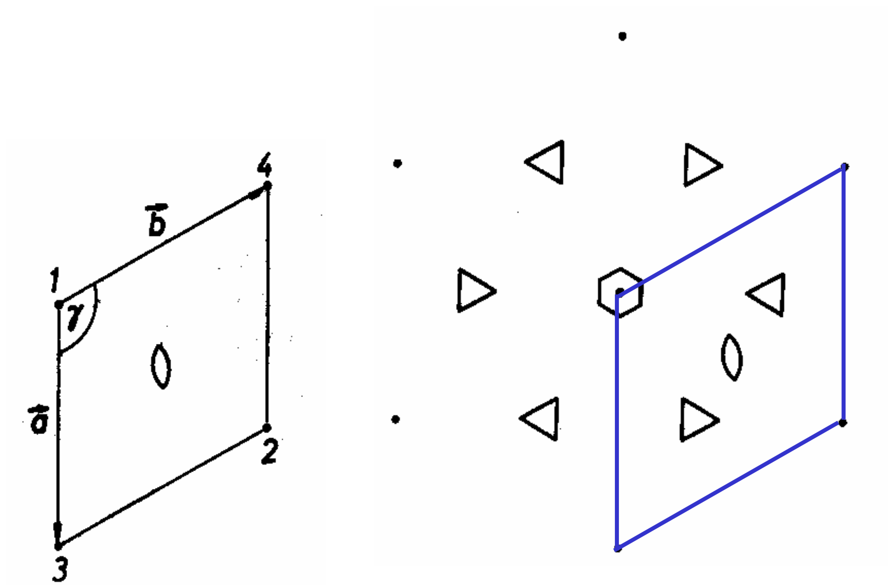
$a_o = b_o \quad \gamma = 120^o$

hexagonal mesh

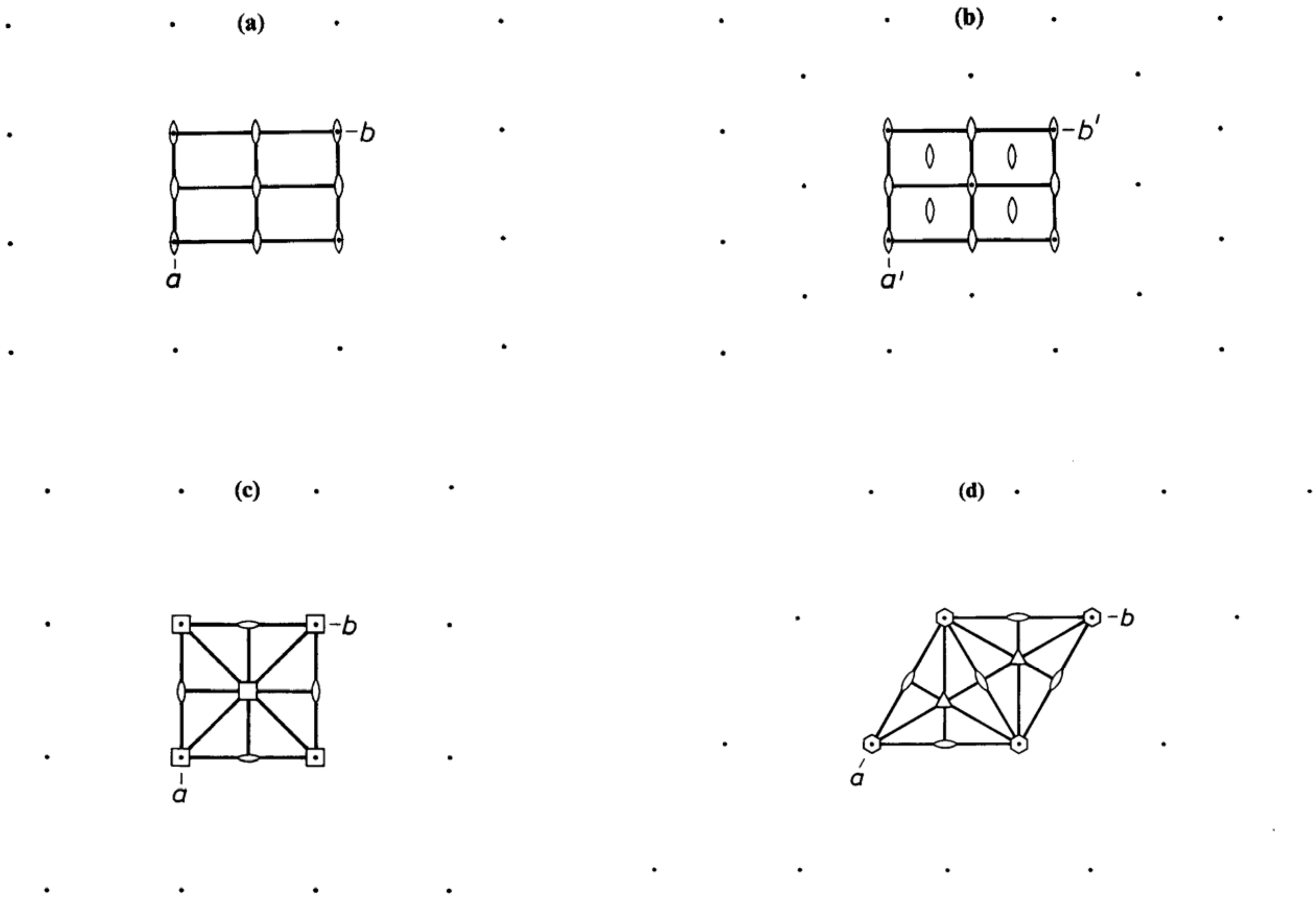
6-fold axis,3-fold axis

mirror plane





Plane Lattice



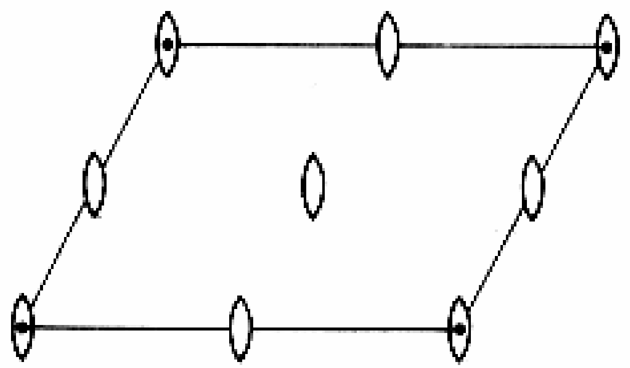
Plane Lattice

		Shape of unit mesh	Lattice parameters	Characteristic symmetry elements
General plane lattices		Parallelogram	$a_0 \neq b_0$ $\gamma \neq 90°$	2
Special plane lattice	a	Rectangle (primitive)	$a_0 \neq b_0$ $\gamma = 90°$	m
	b	Rectangle (centred)	$a_0 \neq b_0$ $\gamma = 90°$	m
	c	Square	$a_0 = b_0$ $\gamma = 90°$	4
	d	120° Rhombus	$a_0 = b_0$ $\gamma = 120°$	6 (3)

Space Lattice

- general lattice (triclinic P-lattice)

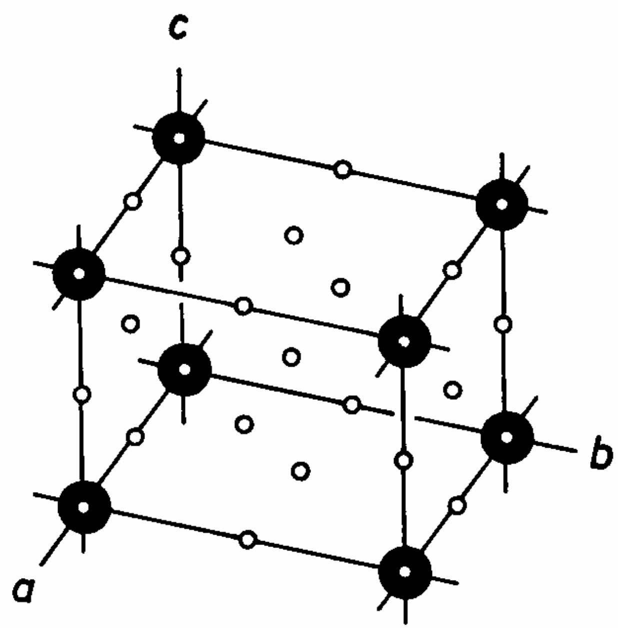
oblique plane lattice



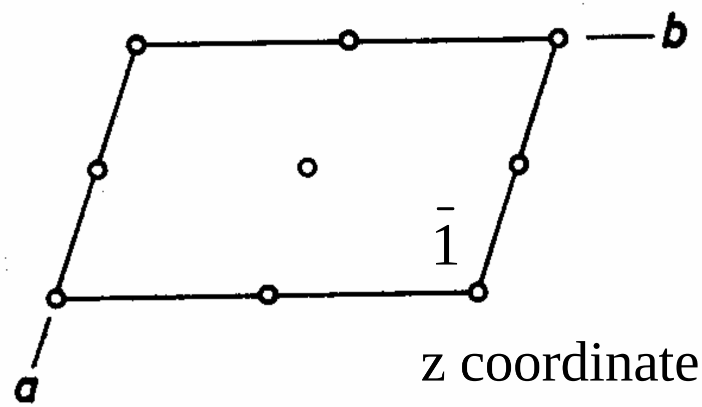
lattice points of stacked plane do not coincide
→ lose 2-fold axis

point group: $\bar{1}$

space group: $P\bar{1}$



(x,y,0 projection)



z coordinate: 0 and $\frac{1}{2}$

$a_o \neq b_o \neq c_o$

$\alpha \neq \beta \neq \gamma \neq 90^o$

Table 8.2. The 32 point groups

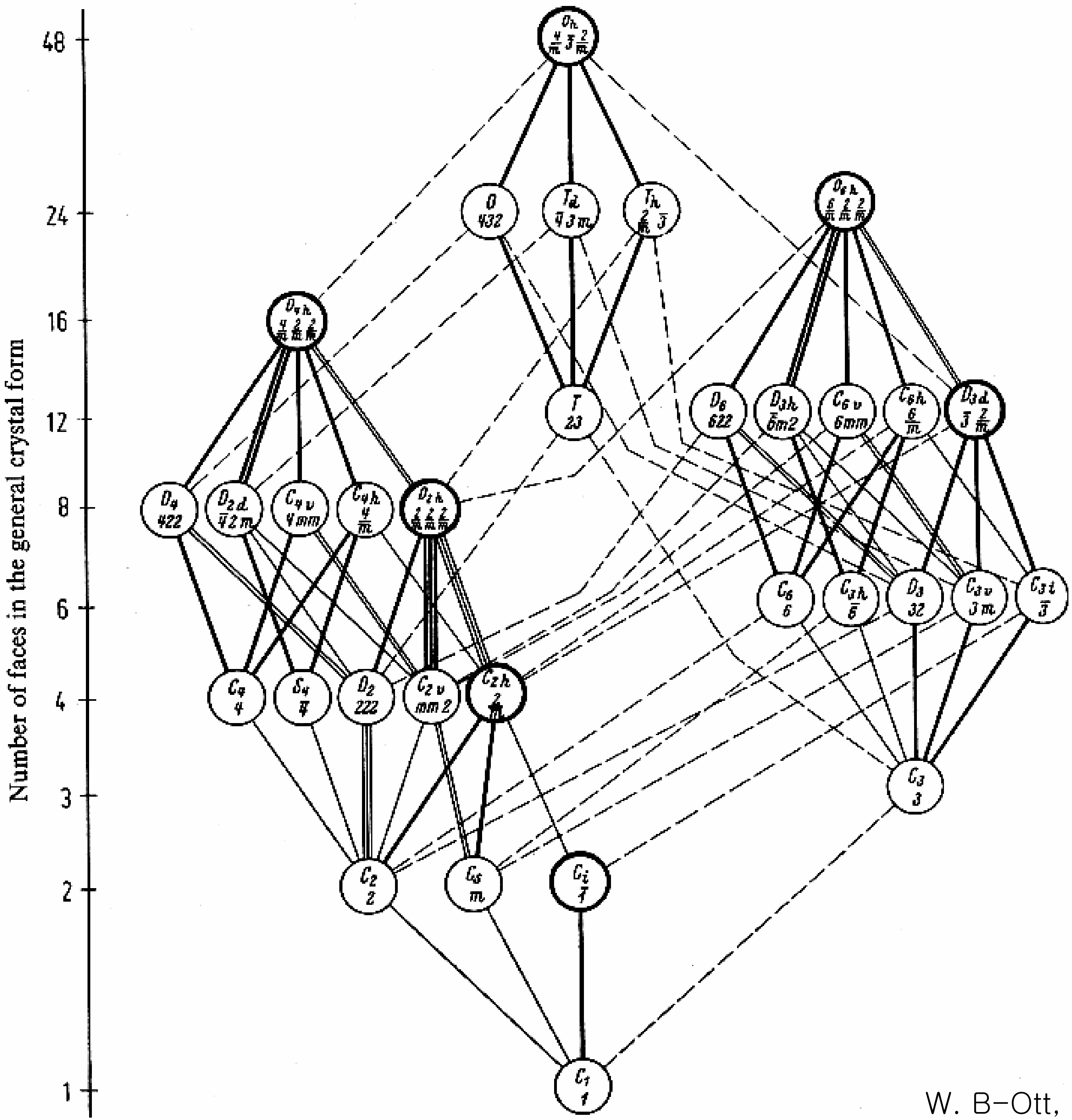
Crystal system	Point groups	
Triclinic	$\bar{1}$	1
Monoclinic	2/m	m, 2
Orthorhombic	2/m 2/m 2/m (mmm)	mm2, 222
Tetragonal	4/m 2/m 2/m (4/mmm)	$\bar{4}$2m, 4mm, 422 4/m, $\bar{4}$, 4
Trigonal	$\bar{3}$ 2/m ($\bar{3}$m)	3m, 32, $\bar{3}$, 3
Hexagonal	6/m 2/m 2/m (6/mmm)	$\bar{6}$m2, 6mm, 622 6/m, $\bar{6}$, 6
Cubic	4/m $\bar{3}$ 2/m (m$\bar{3}$m)	$\bar{4}$3m, 432, 2/m$\bar{3}$, 23 (m$\bar{3}$)

Table 7.1. The seven crystal systems

Crystal system	Restrictions on the axial system
Triclinic	$a \neq b \neq c \quad \alpha \neq \beta \neq \gamma$[a]
Monoclinic	$a \neq b \neq c \quad \alpha = \gamma = 90°, \quad \beta > 90°$
Orthorhombic	$a \neq b \neq c \quad \alpha = \beta = \gamma = 90°$
Tetragonal	$a = b \neq c \quad \alpha = \beta = \gamma = 90°$ $(a_1 = a_2 \neq c)$
Trigonal[b]	$a = b \neq c \quad \alpha = \beta = 90°, \quad \gamma = 120°$ $(a_1 = a_2 \neq c)$
Hexagonal	
Cubic	$a = b = c \quad \alpha = \beta = \gamma = 90°$ $(a_1 = a_2 = a_3)$

Table 7.2. Symmetry directions in the seven crystal systems

	Position in the international symbol		
	1st	2nd	3rd
Triclinic		–	
Monoclinic		b	
Orthorhombic	a	b	c
Tetragonal	c	⟨a⟩	⟨110⟩
Trigonal	c	⟨a⟩	–[c]
Hexagonal	c	⟨a⟩	⟨210⟩
Cubic	⟨a⟩	⟨111⟩	⟨110⟩



W. B-Ott, Crystallography

Space Lattice

– primitive lattice

Shape of unit mesh in stacked layers	Interplanar spacing	Lattice
Parallelogram[a] ($a_0 \neq c_0$)	b_0	Monoclinic P
Rectangle ($a_0 \neq b_0$)	c_0	Orthorhombic P
Square ($a_0 = b_0$)	$c_0 \neq (a_0 = b_0)$	Tetragonal P
Square ($a_0 = b_0$)	$c_0 = (a_0 = b_0)$	Cubic P
120°-Rhombus ($a_0 = b_0$)	c_0	Hexagonal P

[a] Note that for historical reasons, the description $a_0 \neq b_0, \gamma \neq 90°$ has been changed in this case to $a_0 \neq c_0, \beta \neq 90°$.

Space Lattice

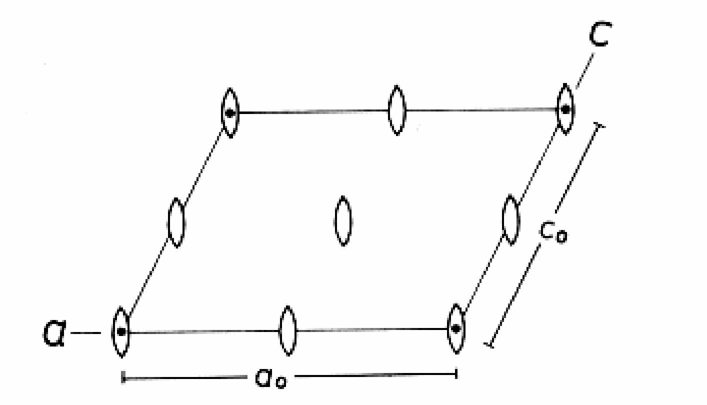
- monoclinic P-lattice

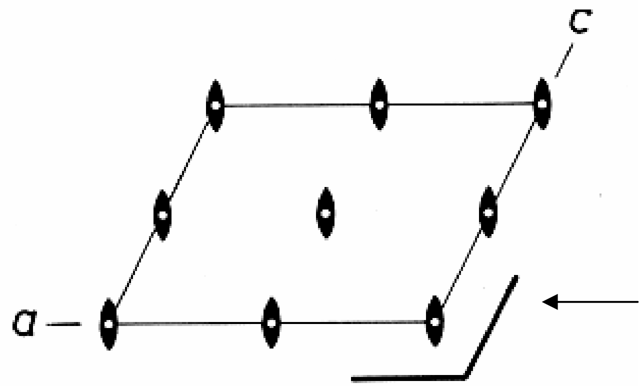
oblique plane lattice

stacking directly above

2-fold axis along $\parallel \vec{b}$

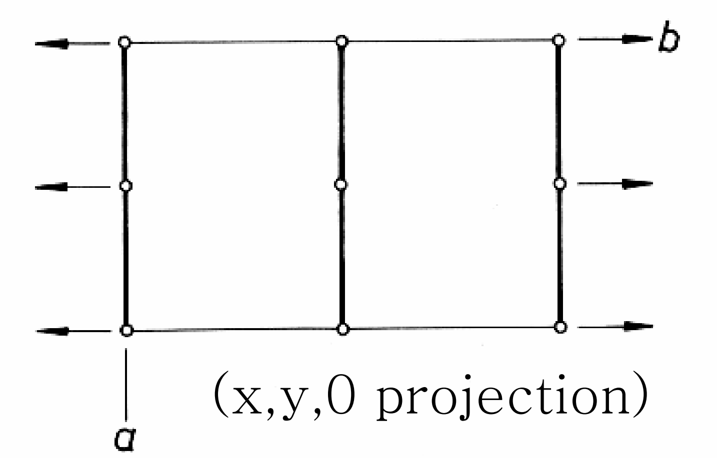
mirror $x, 0, z$ & $x, \frac{1}{2}, z$





Mirror plane b=0 and 1/2

(x,0,z projection)



(x,y,0 projection)

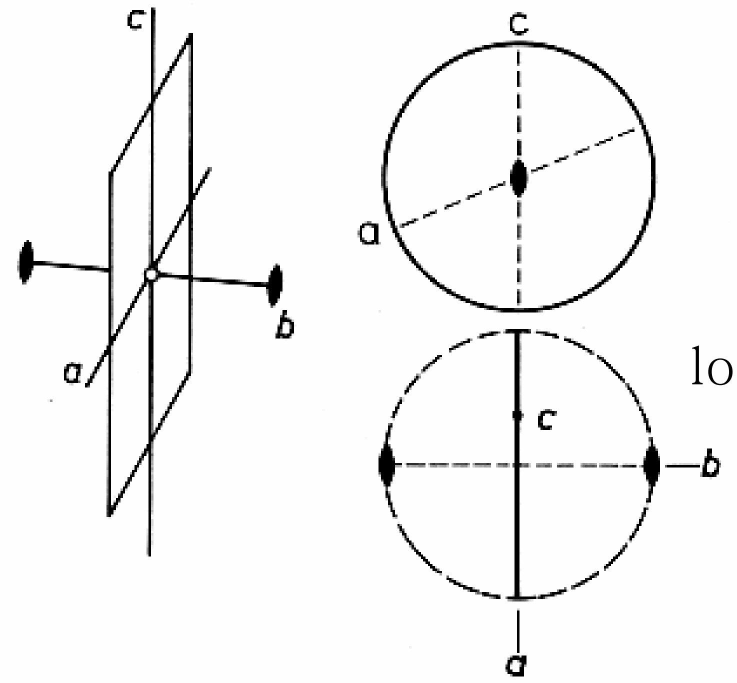
$a_o \neq b_o \neq c_o$

$\alpha = \gamma = 90^o, \ \beta > 90^o$

point group: $\frac{2}{m}$

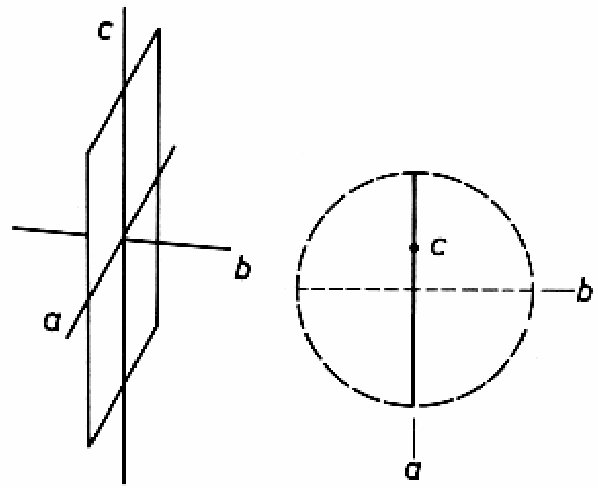
space group: P $\frac{2}{m}$

- monoclinic P-lattice

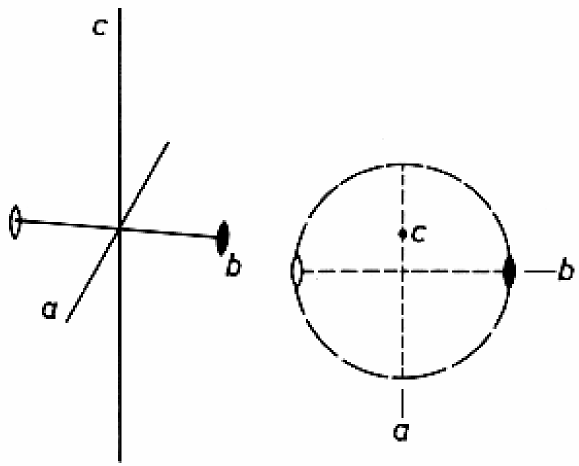


$2/m - C_{2h}$

lower symmetry



$m - C_s$



$2 - C_2$

Space Lattice

- orthorhombic P-lattice

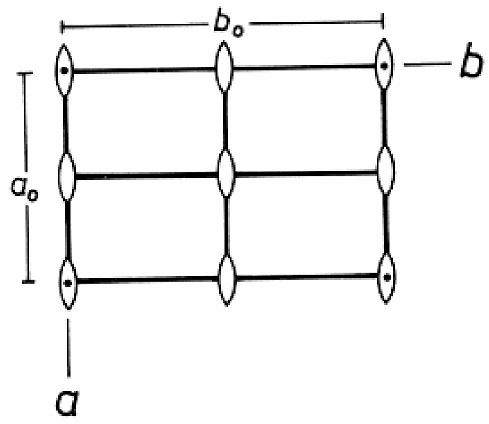
  rectangular plane lattice   stacking directly above

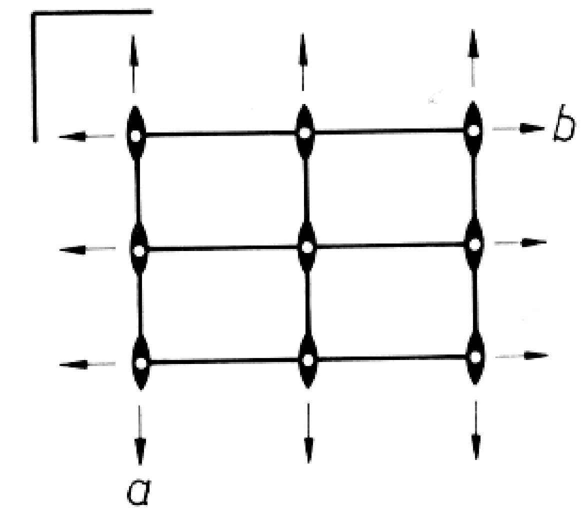
  2-fold axis $\parallel \vec{c}$

  mirror plane $x, y, 0$ & $x, y, ½$

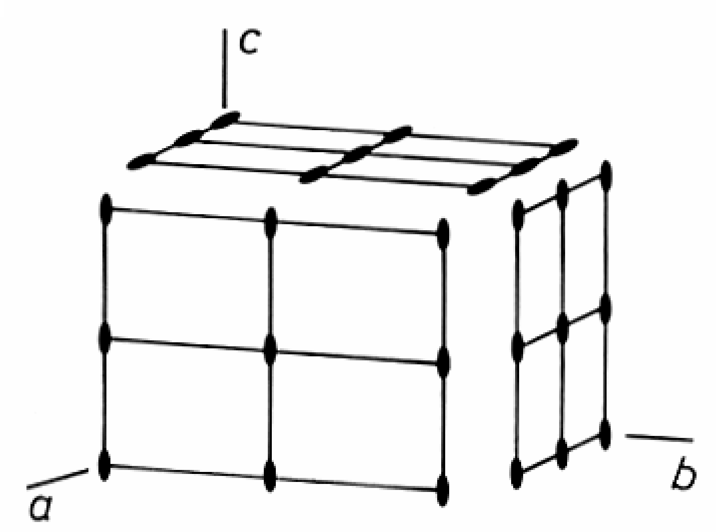
  2-fold axis $x,0,0$ $x,0,½$ $x,½,o$ $x,½,½$ $\perp$ mirror

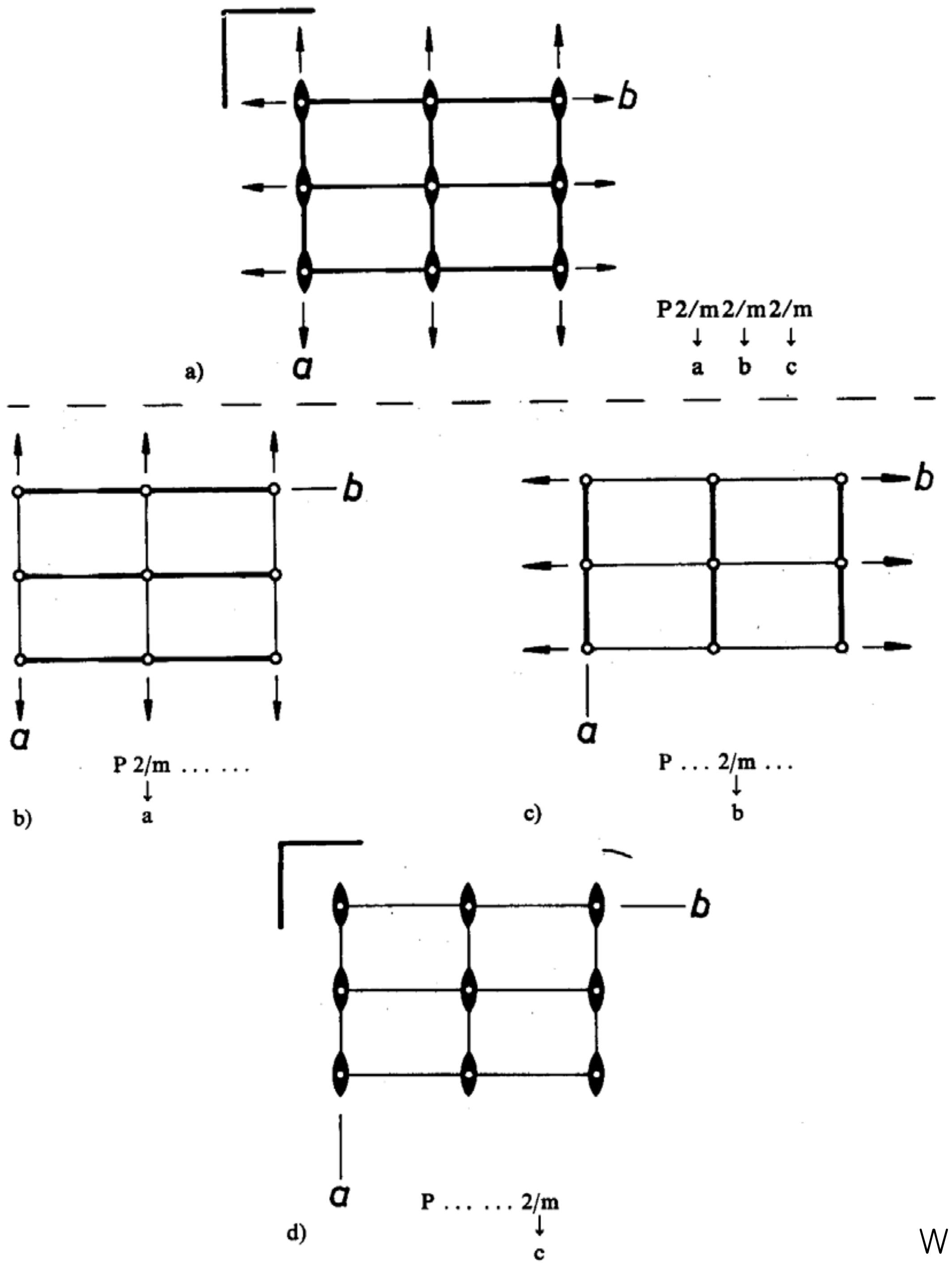
  $0,y,0$ $0,y,½$ $½,y,0$ $½,y,½$





(x,y,0 projection)




b
a
a)
P 2/m 2/m 2/m
a b c
b
a
b)
P 2/m . . . . . .
a
b
a
c)
P . . . 2/m . . .
b
b
a
d)
P 2/m
c

Space Lattice

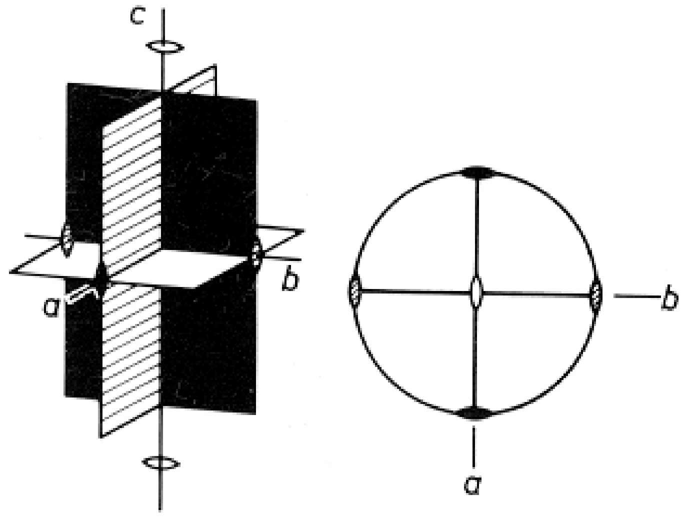
- orthorhombic P-lattice

$$a_o \neq b_o \neq c_o$$

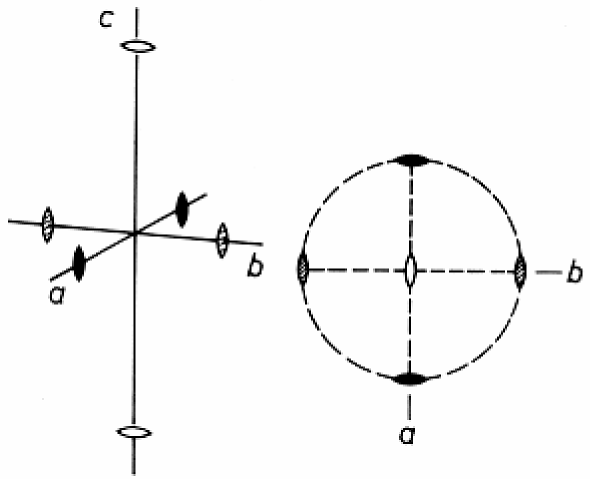
$$\alpha = \beta = \gamma = 90^o$$

point group: $\frac{2}{m}\frac{2}{m}\frac{2}{m}$

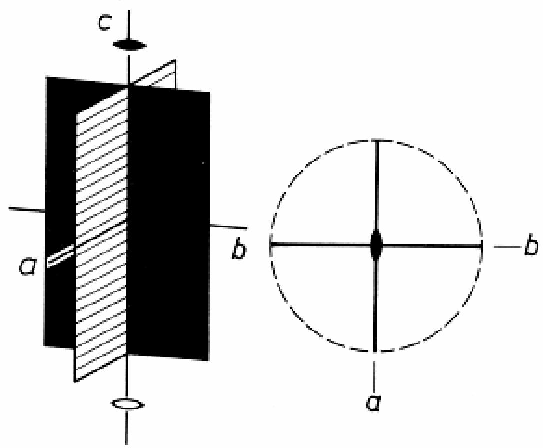
space group: $P\frac{2}{m}\frac{2}{m}\frac{2}{m}$



2/m 2/m 2/m – D_{2h}



222 – D_2



mm2 – C_{2v}

Space Lattice

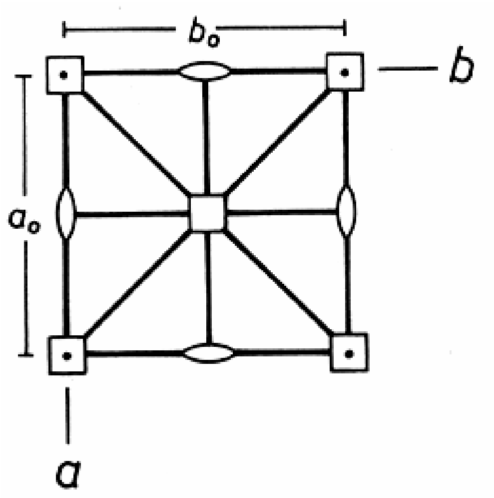
- tetragonal P-lattice

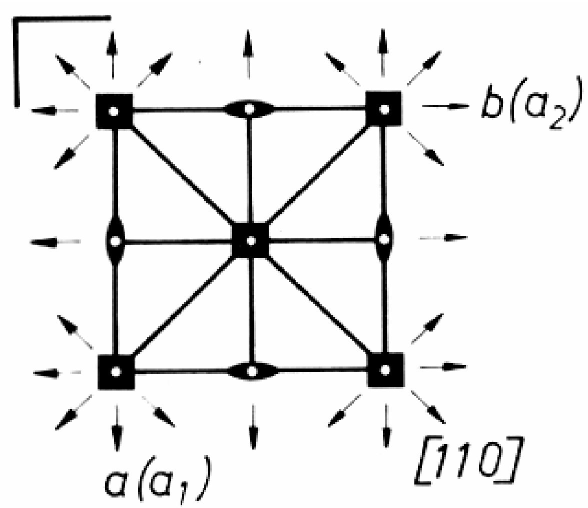
square plane lattice- stacking directly above $a_o = b_o \neq c_o$

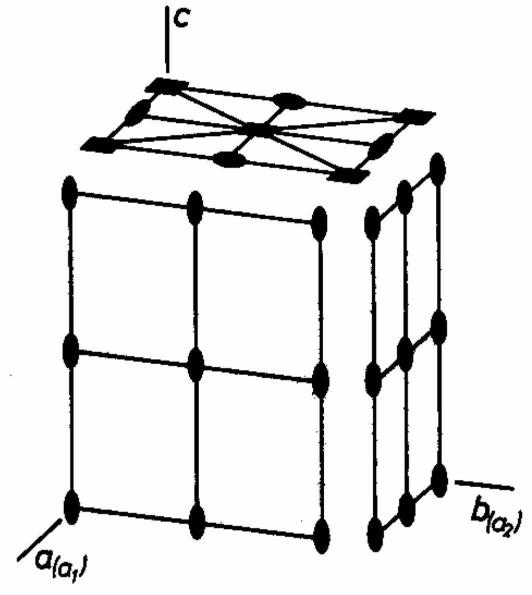
4-fold axis $\parallel \vec{c}$ mirror plane $x, y, 0$ & $x, y, \frac{1}{2}$

2-fold axis $\parallel \vec{a}$ $\parallel \vec{b}$ $\perp$ mirror plane

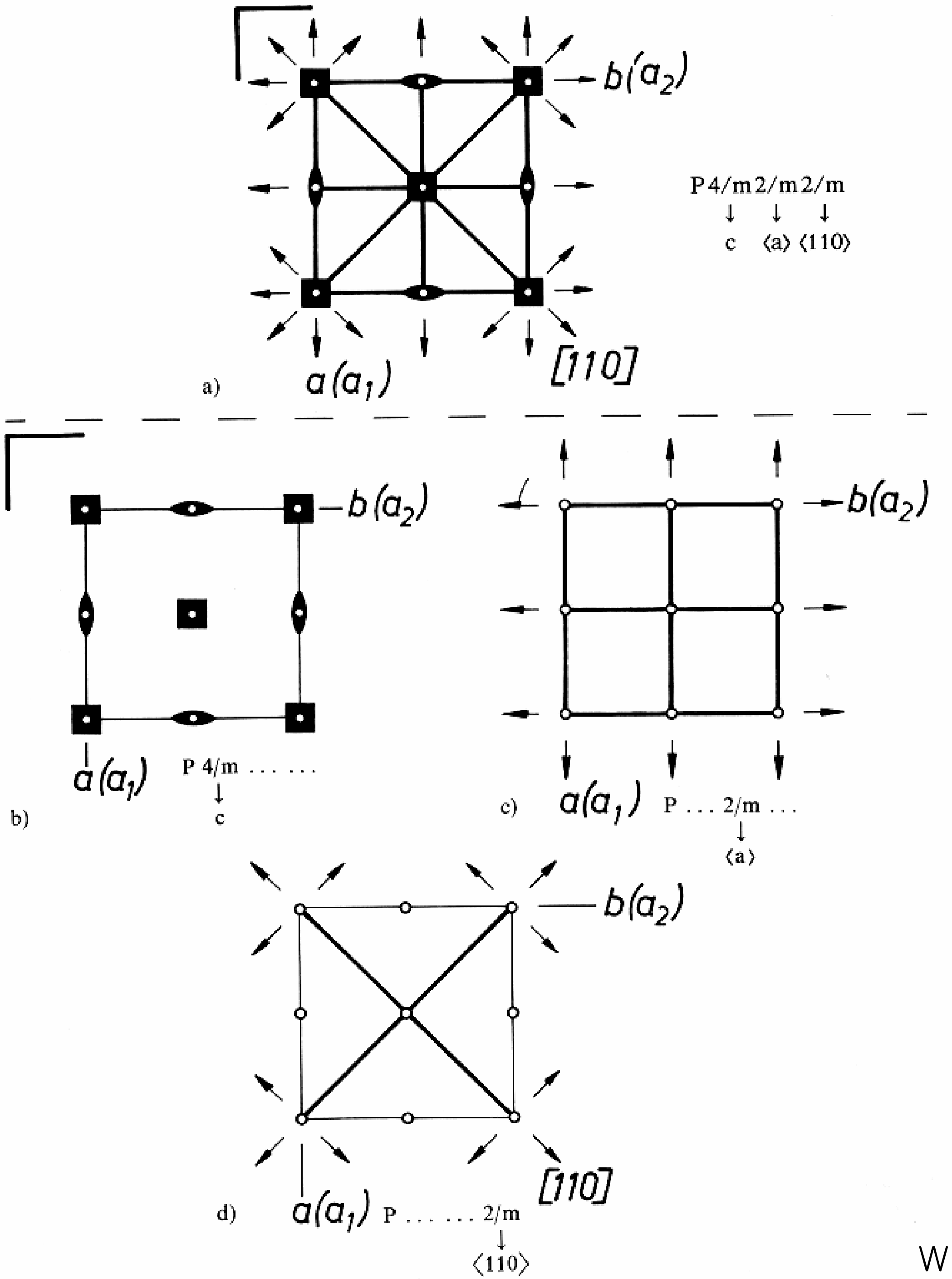
2-fold axis $<110>$ $\perp$ mirror plane







*glide plane, screw axis


b(a2)
P 4/m 2/m 2/m
c ⟨a⟩ ⟨110⟩
a)
a(a1)
[110]
b(a2)
a(a1)
P 4/m . . . . . .
c
b)
b(a2)
c)
a(a1)
P . . . 2/m . . .
⟨a⟩
b(a2)
d)
a(a1)
P 2/m
⟨110⟩
[110]

Space Lattice

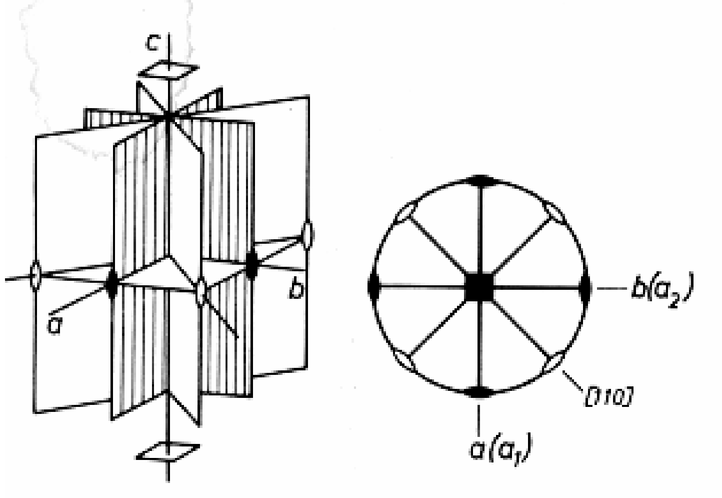
- tetragonal P-lattice

$$a_o = b_o \neq c_o$$

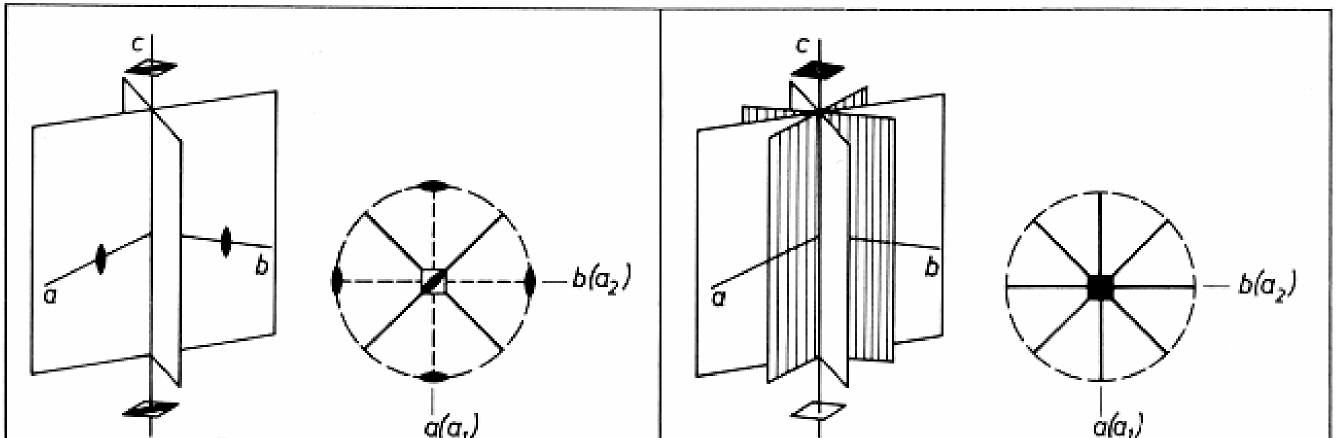
$$\alpha = \beta = \gamma = 90^o$$

point group: $\frac{4}{m}\frac{2}{m}\frac{2}{m}$

space group: $P\frac{4}{m}\frac{2}{m}\frac{2}{m}$



4/m 2/m 2/m – D_{4h}

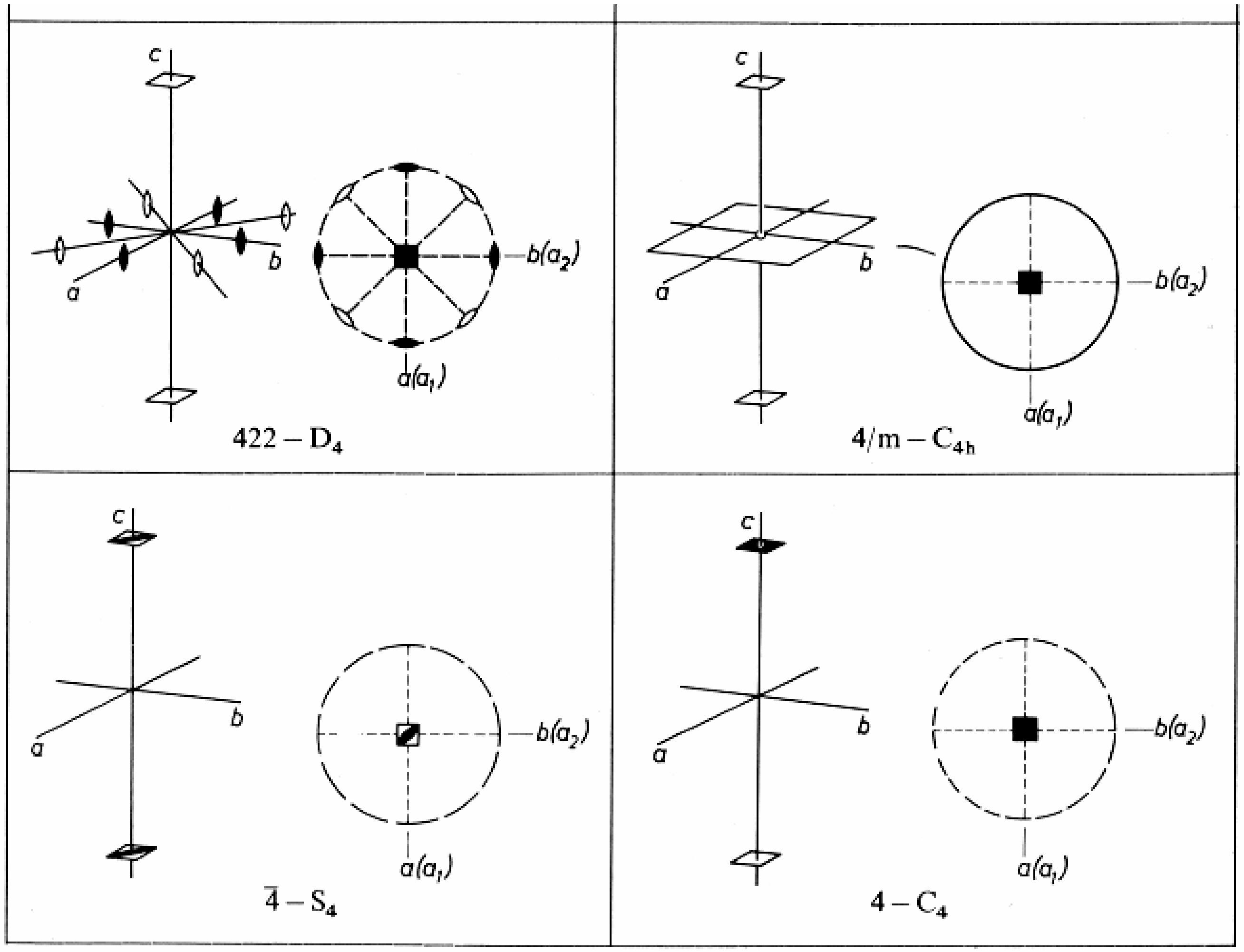


$\bar{4}2m$ – D_{2d}

4mm – C_{4v}

Space Lattice

- tetragonal P-lattice



Space Lattice

-hexagonal P-lattice

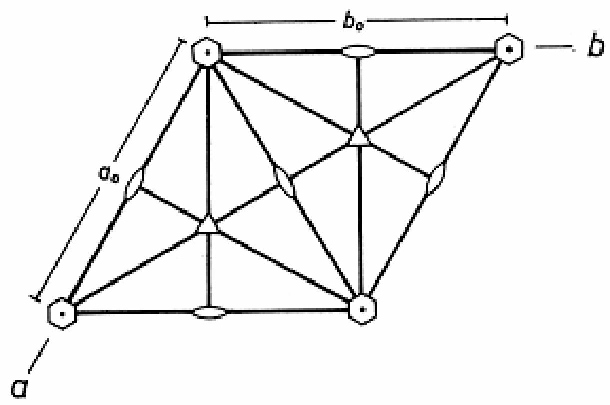
hexagonal plane lattice- stacking directly above

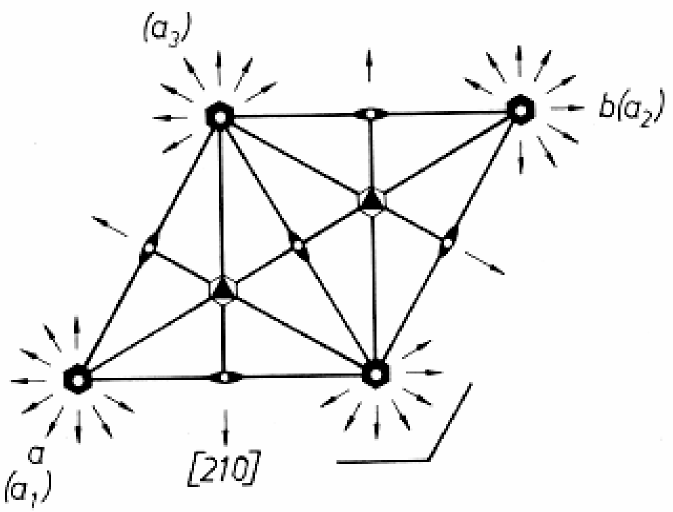
$$a_o = b_o \neq c_o$$

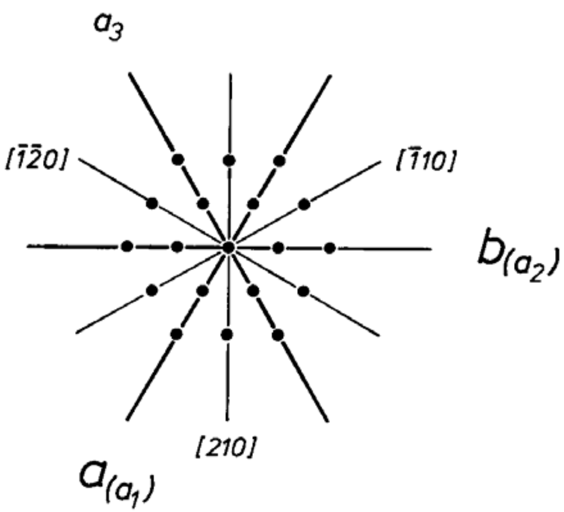
6-fold axis $\parallel \vec{c}$ $\perp$ mirror plane $x, y, 0$ & $x, y, \frac{1}{2}$

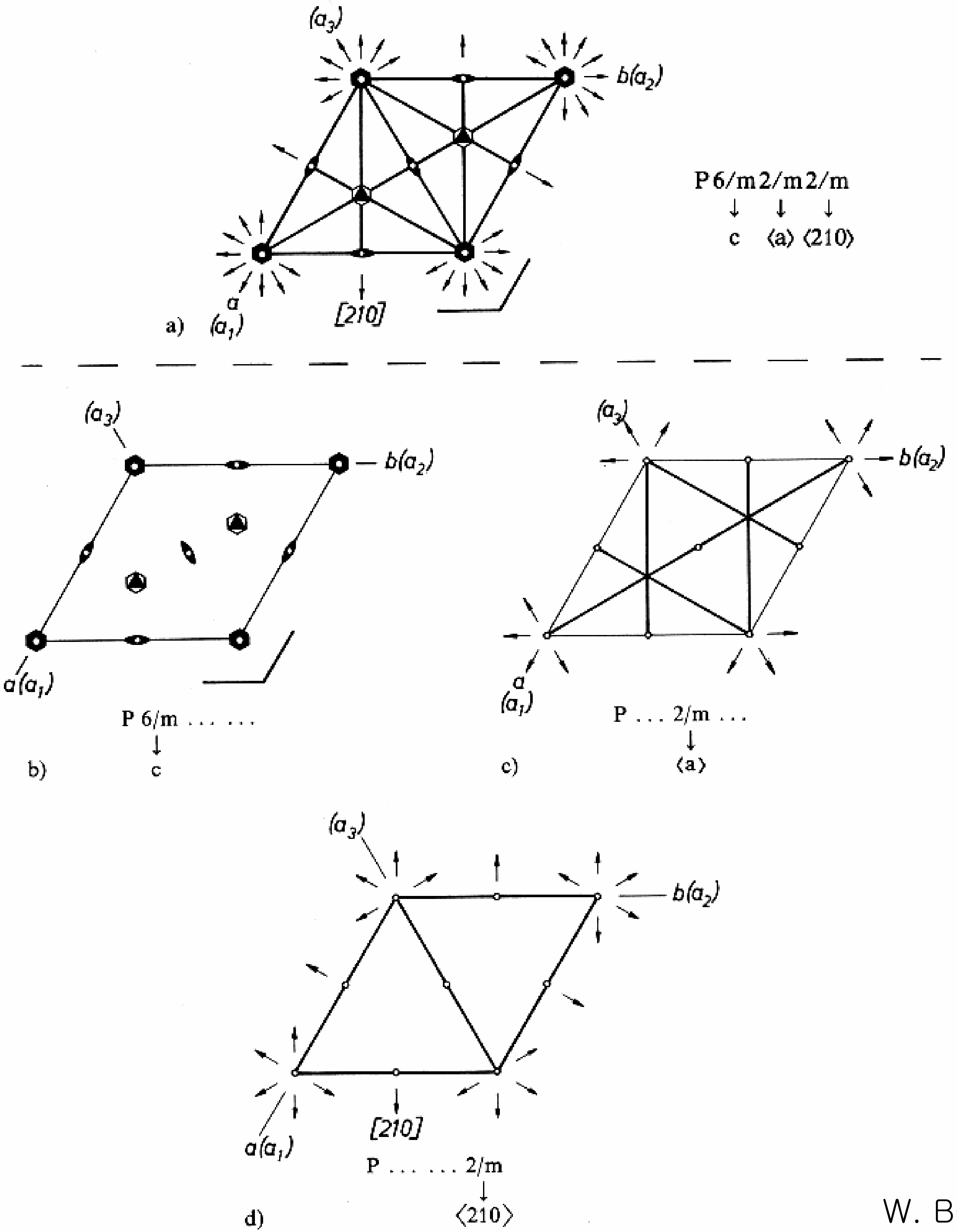
2-fold axis $\parallel \vec{a}$ $\parallel \vec{b}$ $\perp$ mirror plane

2-fold axis $<210>$ $\perp$ mirror plane








(a3)
b(a2)
P6/m2/m2/m
c ⟨a⟩ ⟨210⟩
a) a (a1)
[210]
(a3)
b(a2)
a(a1)
P 6/m . . . . . .
c
b)
(a3)
b(a2)
a (a1)
P . . . 2/m . . .
⟨a⟩
c)
(a3)
b(a2)
a(a1)
[210]
P 2/m
⟨210⟩
d)

Space Lattice

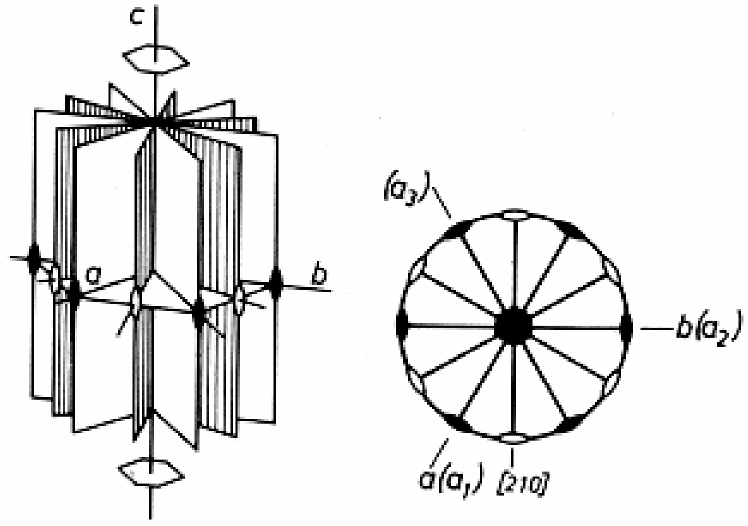
- hexagonal P-lattice

$$a_o = b_o \neq c_o$$

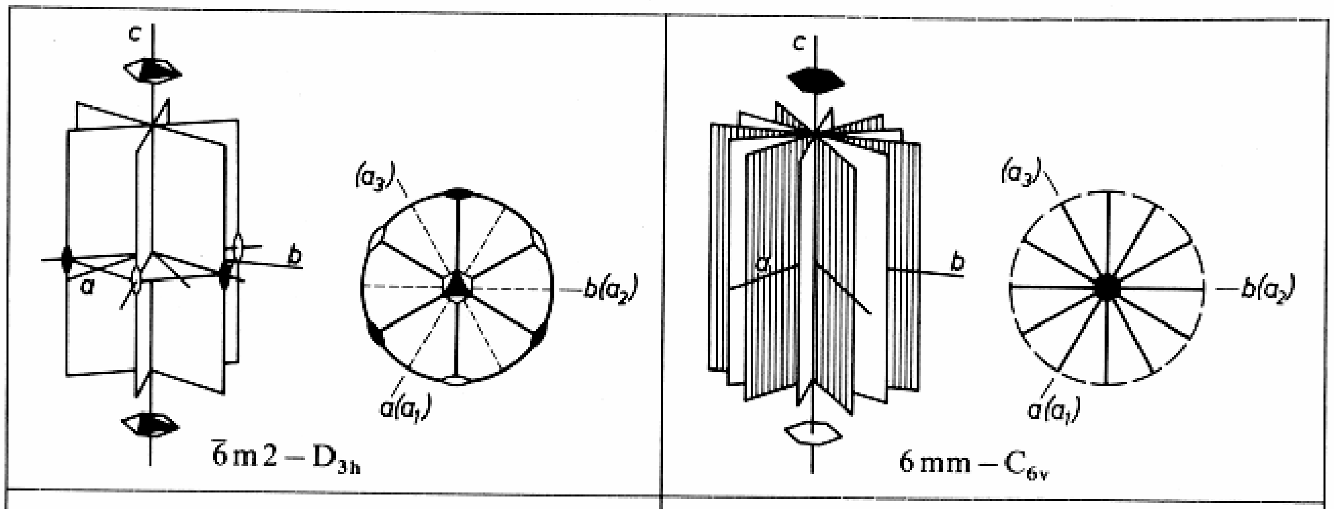
$$\alpha = \beta = 90^{o}, \gamma = 120^{o}$$

point group: $\frac{6}{m}\frac{2}{m}\frac{2}{m}$

space group: P $\frac{6}{m}\frac{2}{m}\frac{2}{m}$



6/m 2/m 2/m – D_{6h}

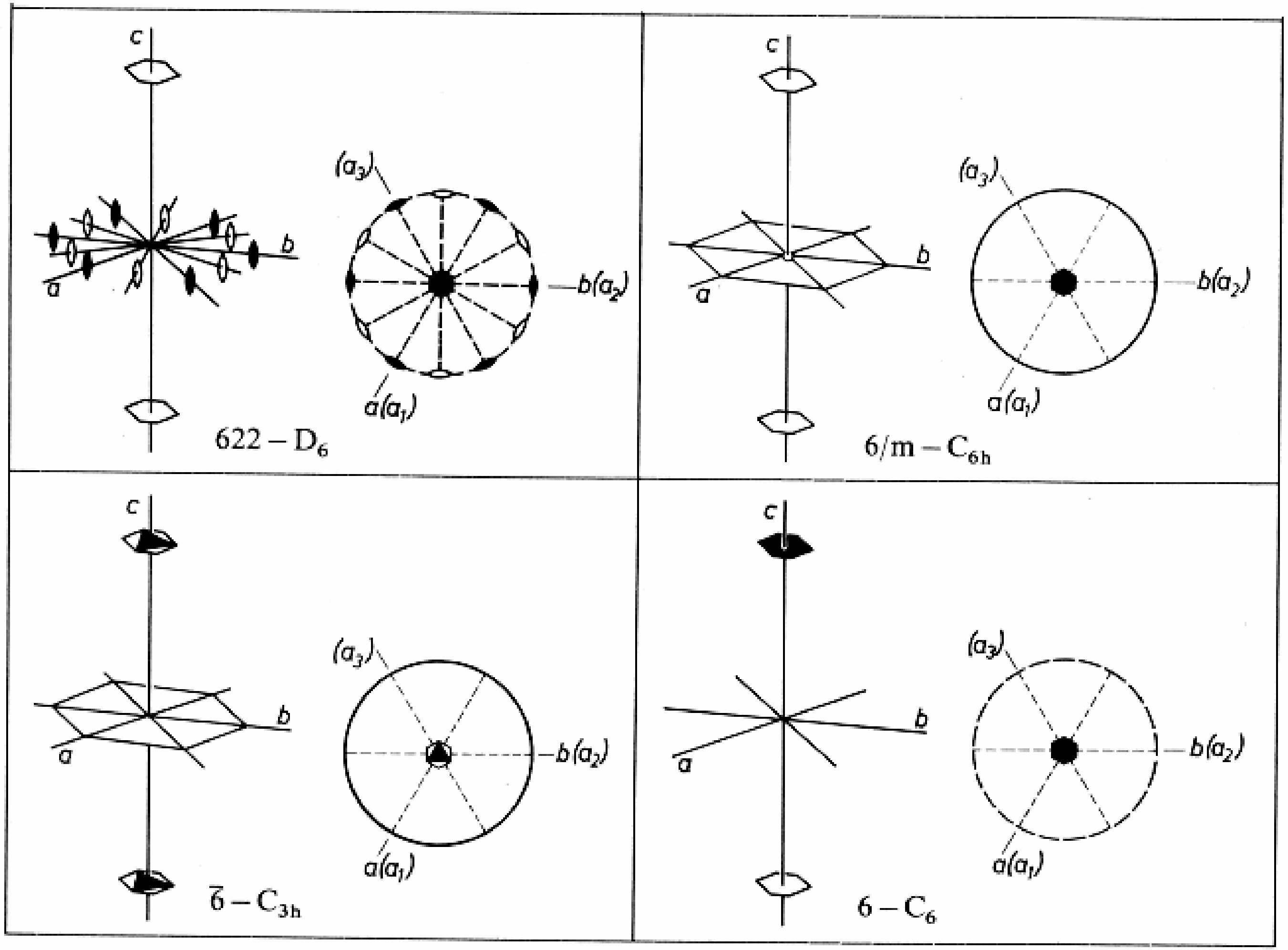


$\bar{6}$m2 – D_{3h}

6mm – C_{6v}

Space Lattice

- hexagonal P-lattice



Space Lattice

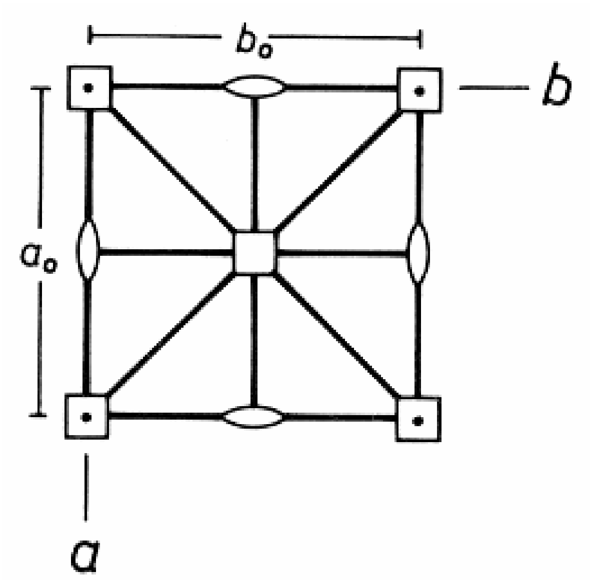
-cubic P-lattice

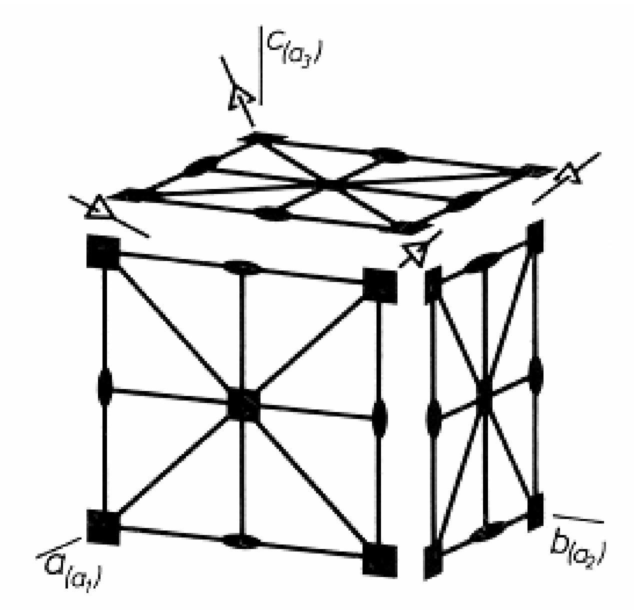
square plane lattice- stacking directly above $a_o = b_o = c_o$

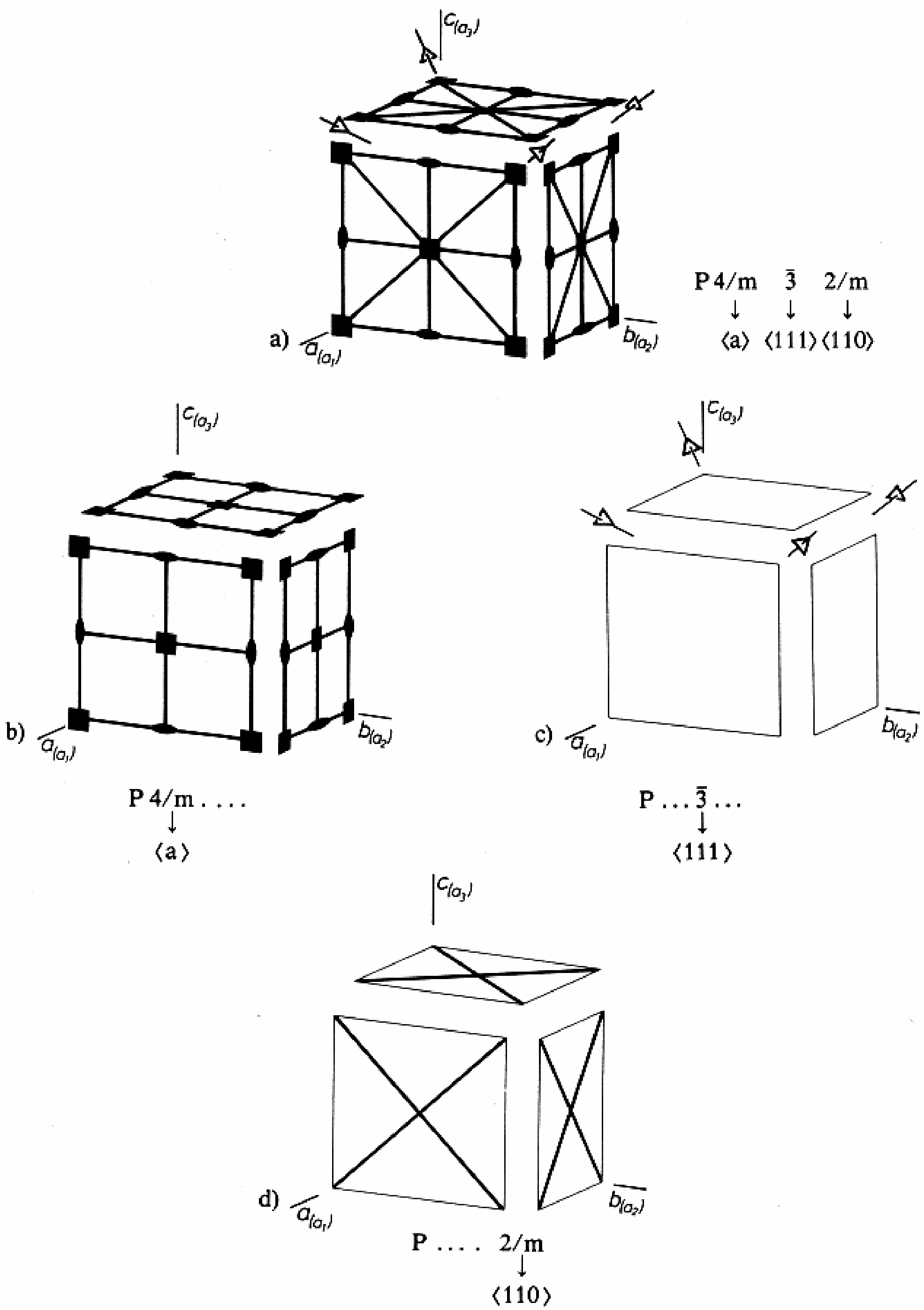
4-fold axis $\parallel \vec{c} \parallel \vec{a} \parallel \vec{b}$ $\perp$ mirror plane

3-fold axis $<111>$

2-fold axis $<110>$ $\perp$ mirror plane






a)
$c_{(a_3)}$
$a_{(a_1)}$
$b_{(a_2)}$
P 4/m $\bar{3}$ 2/m
⟨a⟩ ⟨111⟩ ⟨110⟩
b)
P 4/m . . . .
⟨a⟩
c)
P . . . $\bar{3}$ . . .
⟨111⟩
d)
P 2/m
⟨110⟩

Space Lattice

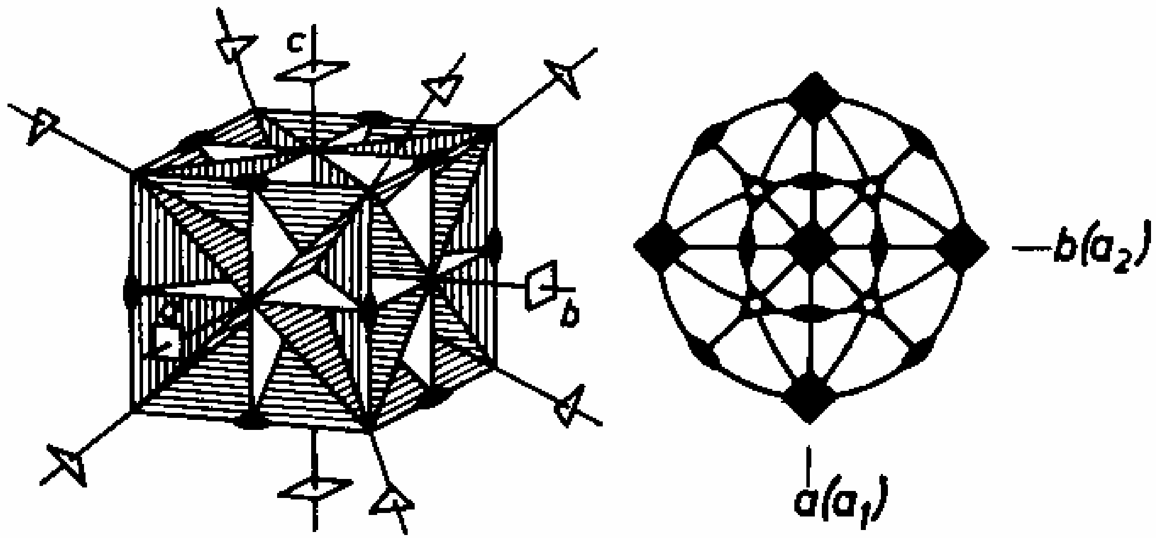
- cubic P-lattice

$a_o = b_o \neq c_o$

$\alpha = \beta = \gamma = 90^o$

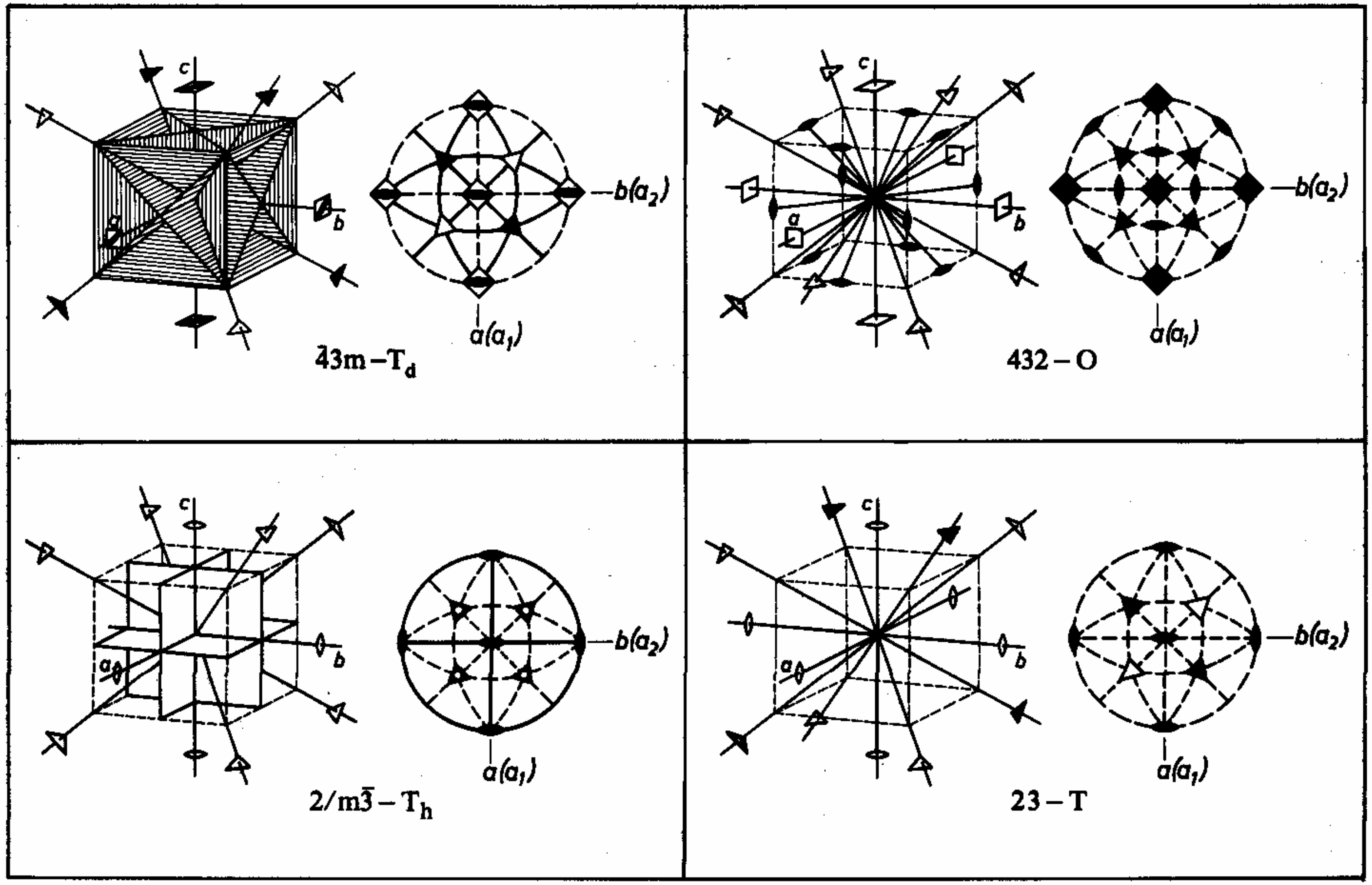
point group: $\frac{4}{m}\bar{3}\frac{2}{m}$

space group: P $\frac{4}{m}\bar{3}\frac{2}{m}$



4/m $\bar{3}$ 2/m – O_h

- cubic P-lattice



Space Lattice

–trigonal lattice

hexagonal plane lattice

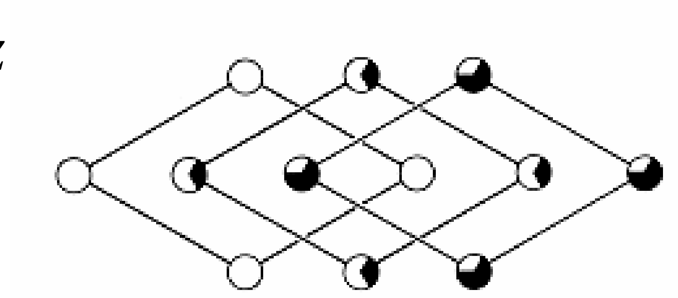
second plane $\frac{1}{3}c_o$ with a lattice point on 3–fold at $\frac{2}{3},\frac{1}{3},z$

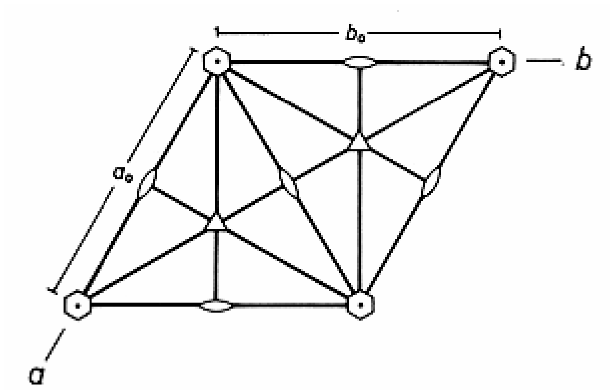
third plane $\frac{2}{3}c_o$ with a lattice point on 3–fold at $\frac{1}{3},\frac{2}{3},z$

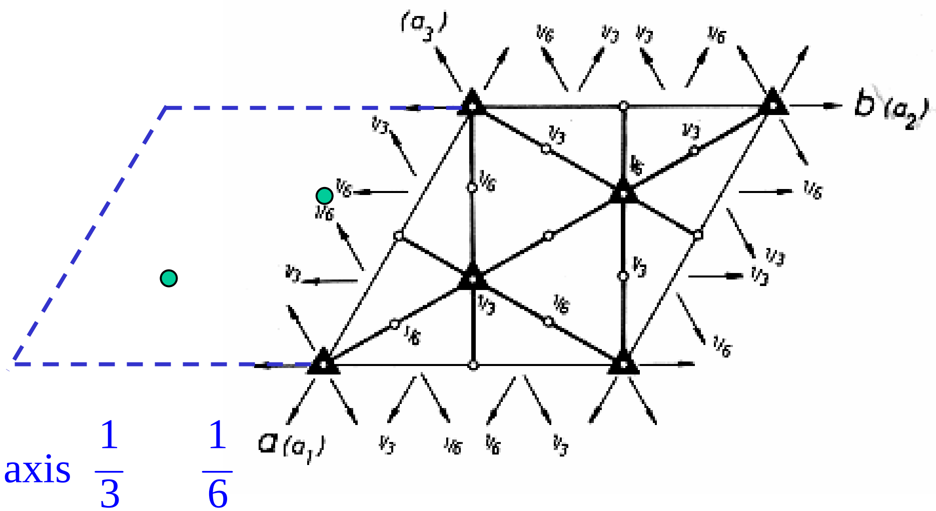
reduce 6–fold to 3–fold axis

remove mirrors $x,0,z;\ 0,y,z;\ x,x,z$

remove 2–fold axis $\parallel \vec{c}$



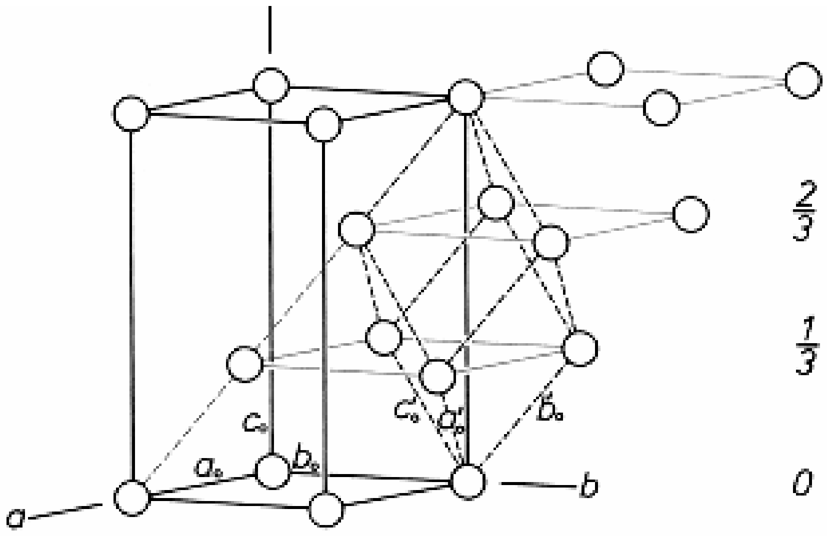


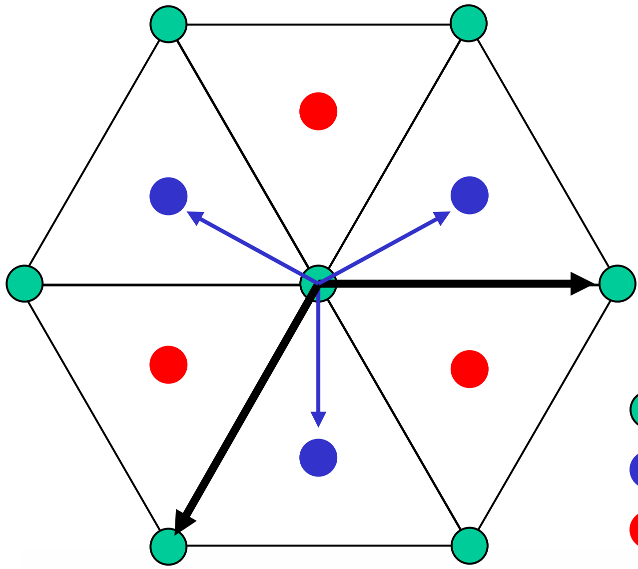


2-fold axis $\frac{1}{3}$ $\frac{1}{6}$

Space Lattice

- trigonal lattice





Trigonal R-lattice

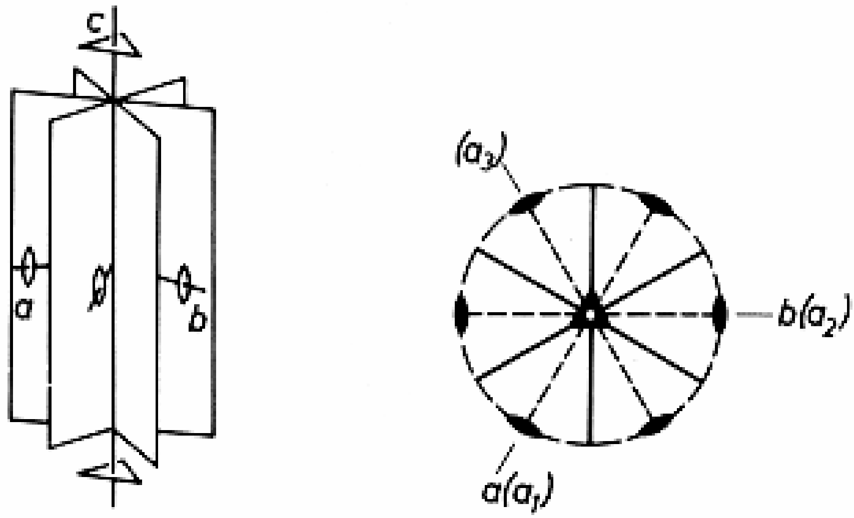
$$a_o = b_o \neq c_o$$

$$\alpha = \beta = 90^o \quad \gamma = 120^o$$

Rhombohedral P-lattice

$$a_o' = b_o' = c_o'$$

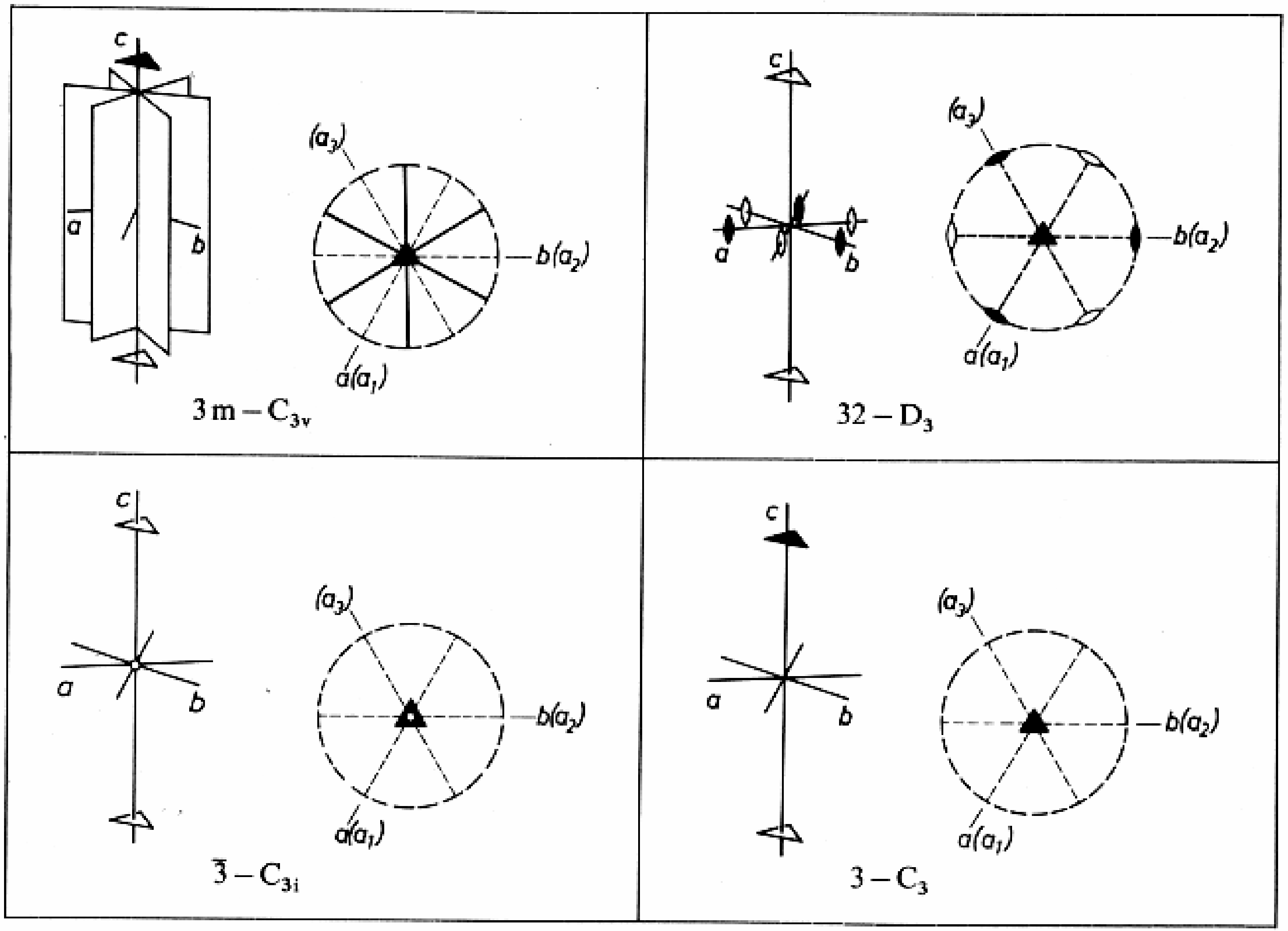
$$\alpha = \beta = \gamma$$



$\bar{3}\ 2/m - D_{3d}$

Space Lattice

– trigonal lattice



Space Lattice

-centered lattice

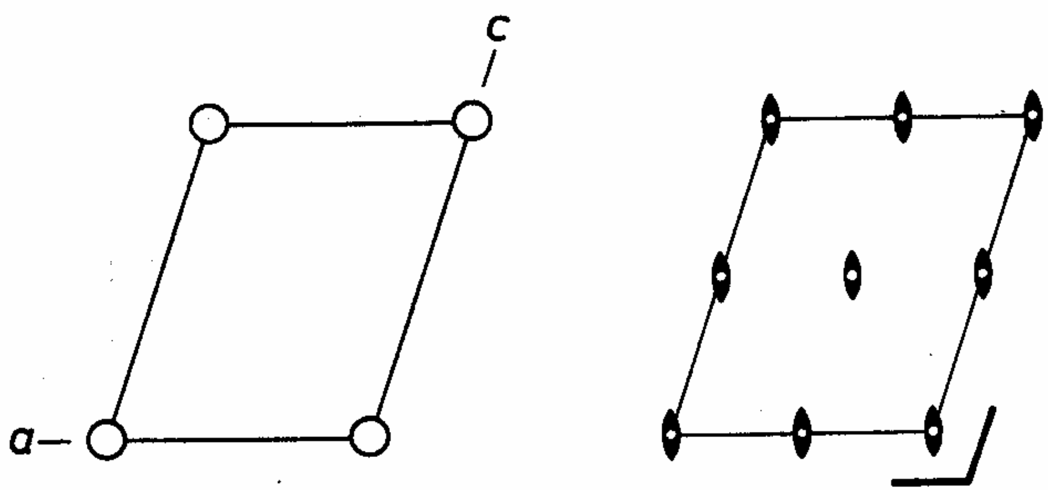
monoclinic P-lattice

lattice point: $\frac{2}{m}$

new lattice point: $\frac{2}{m}$ $\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2};$

$\frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2};$

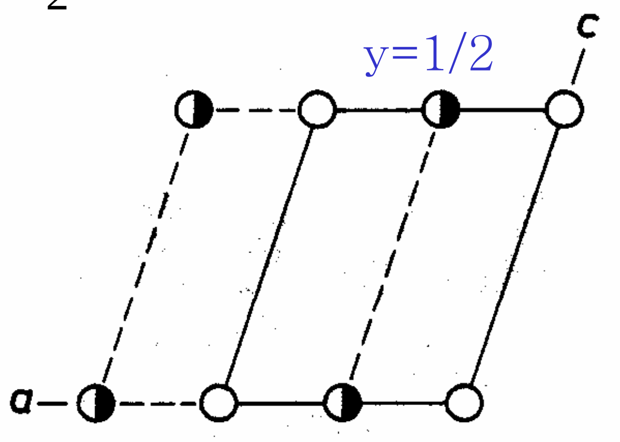
$\frac{1}{2},\frac{1}{2},\frac{1}{2}$



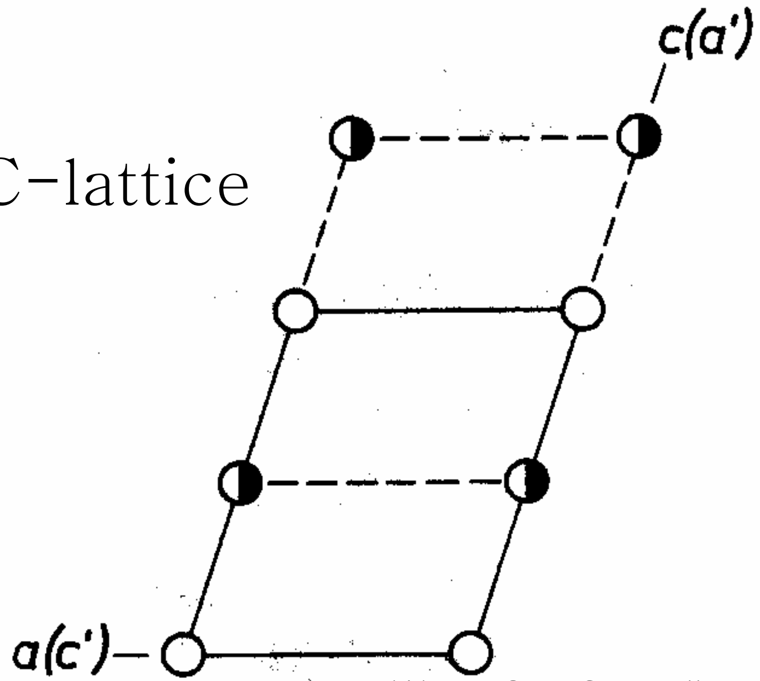
Space Lattice

– monoclinic lattice

a) at $\frac{1}{2},\frac{1}{2},0$ → C–centered lattice or C–lattice



b) at $0,\frac{1}{2},\frac{1}{2}$ → A–lattice → C–lattice



W. B–Ott, Crystallography

Space Lattice

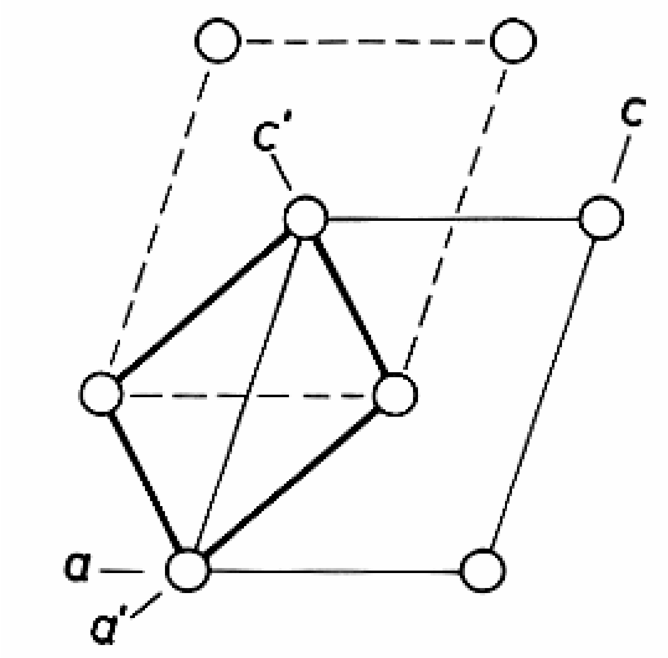
- monoclinic lattice

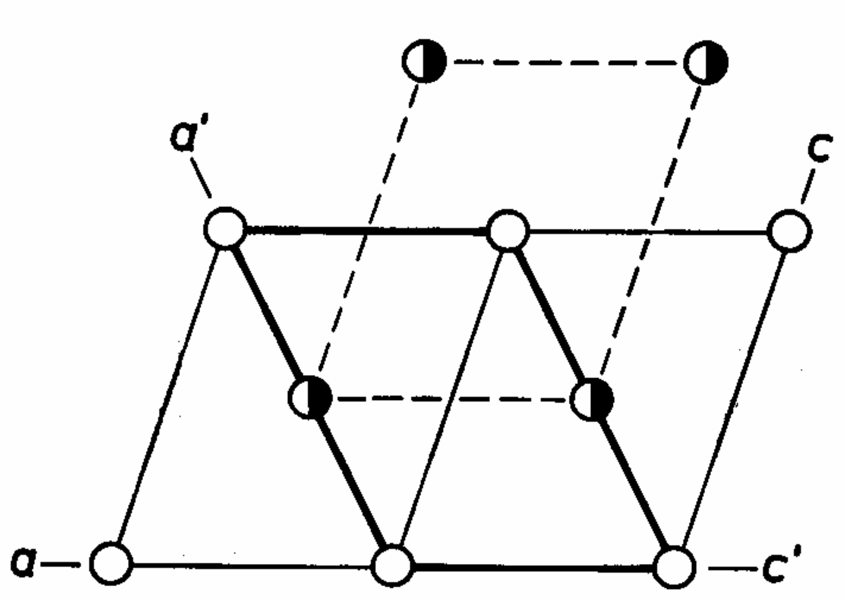
(c) at $\frac{1}{2}, 0, \frac{1}{2}$ → B-lattice

→ smaller primitive unit cell

(d) at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ → I-lattice

→ C-lattice





Space Lattice

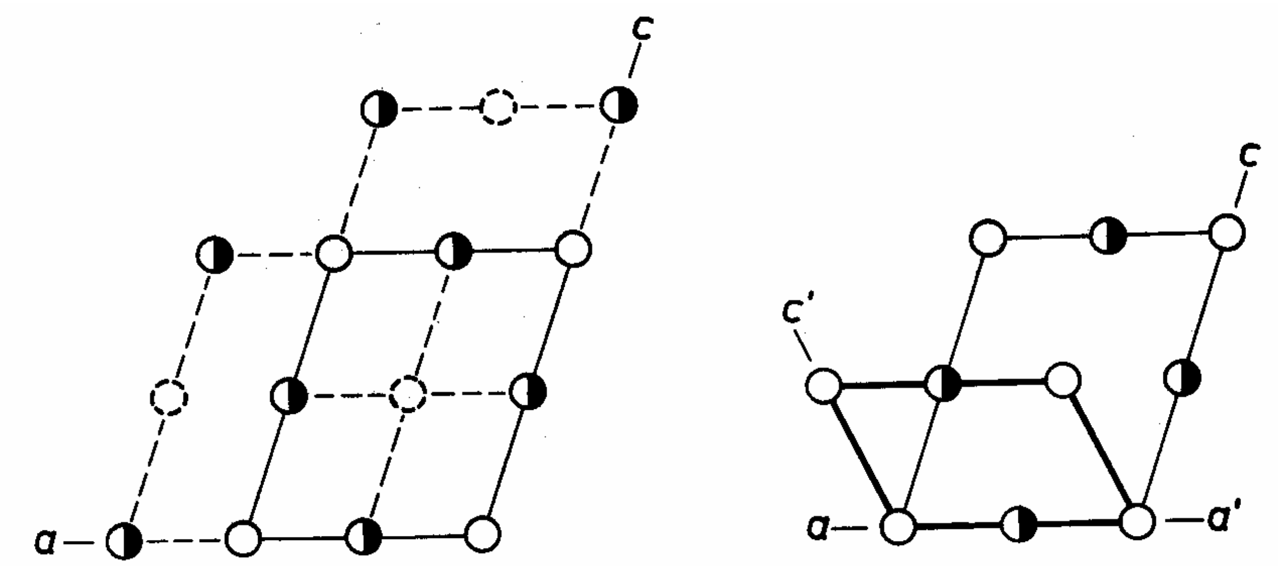
- monoclinic lattice

(e) at $\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$

→ half the cell

(f) at $\frac{1}{2},\frac{1}{2},0;\ 0,\frac{1}{2},\frac{1}{2}$ → further lattice point $\frac{1}{2},0,\frac{1}{2}$

F-lattice → reduced to C-lattice

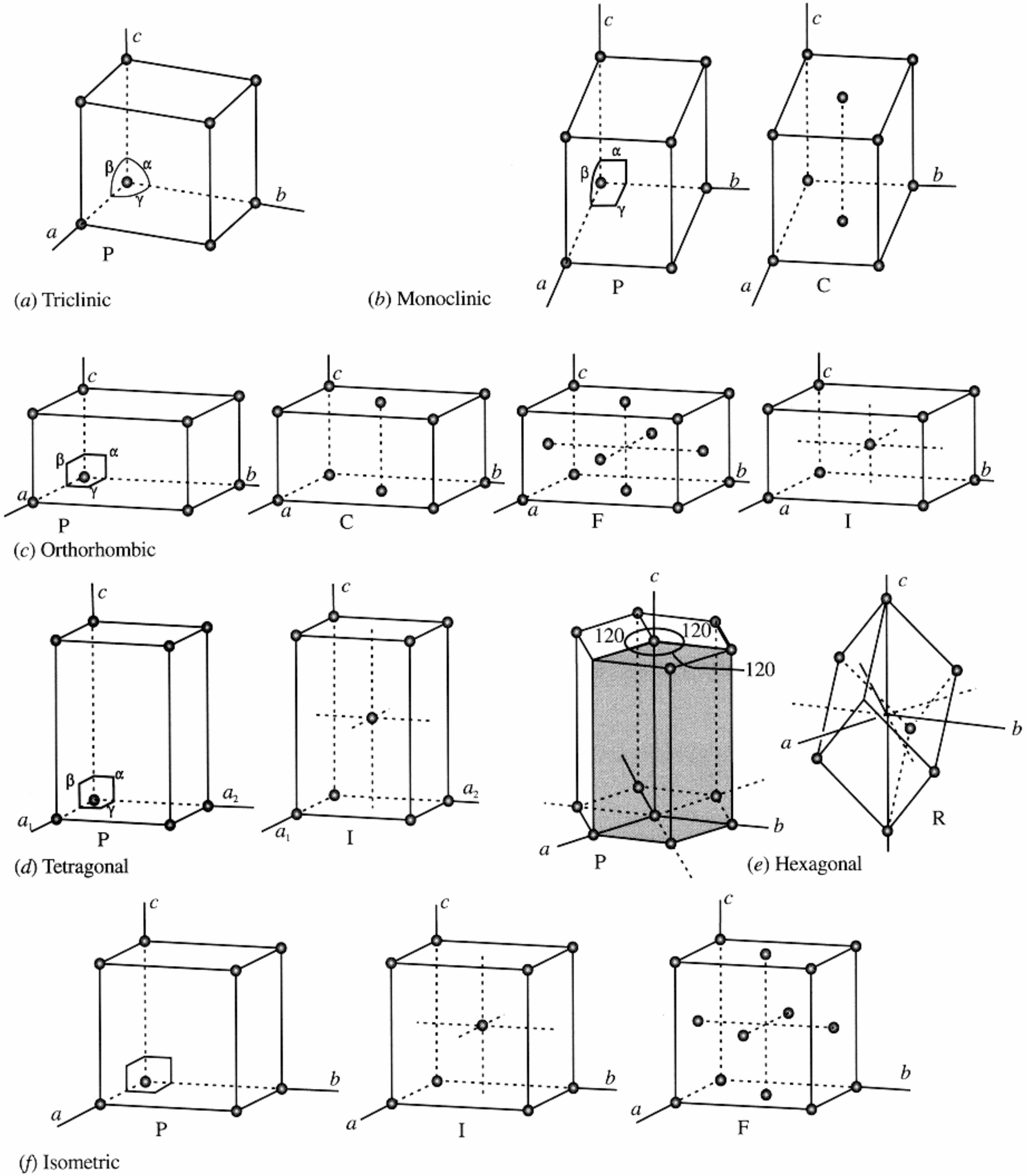


Space Lattice

- 14 Bravais lattice

	P	C	I	F
Triclinic	$P\bar{1}$			
Monoclinic	P 2/m	C 2/m		
Orthorhombic	P 2/m 2/m 2/m	C 2/m 2/m 2/m	I 2/m 2/m 2/m	F 2/m 2/m 2/m
Tetragonal	P 4/m 2/m 2/m		I 4/m 2/m 2/m	
Trigonal	P 6/m 2/m 2/m	$R\bar{3}$ 2/m		
Hexagonal				
Cubic	P 4/m $\bar{3}$ 2/m		I 4/m $\bar{3}$ 2/m	F 4/m $\bar{3}$ 2/m

The 14 Bravais lattice represent the 14 and only way in which it is possible to fill space by a three-dimensional periodic array of points.


(a) Triclinic
(b) Monoclinic
(c) Orthorhombic
(d) Tetragonal
(e) Hexagonal
(f) Isometric
P
C
F
I
R
120
a
b
c
α
β
γ

Space Lattice

- 14 Bravais lattice

Lattice	No. of lattice points in unit cell	Coordinates of lattice points in unit cell
P	1	0,0,0
A	2	0,0,0; $0,\frac{1}{2},\frac{1}{2}$
B	2	0,0,0; $\frac{1}{2},0,\frac{1}{2}$
C	2	0,0,0; $\frac{1}{2},\frac{1}{2},0$
I	2	0,0,0; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$
R	3	0,0,0; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$
F	4	0,0,0; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$

Transformation of Coordinate System

- old axis unit vector a, b, c
  new axis unit vector a', b', c'

$$a' = p_{11}a + p_{12}b + p_{13}c$$
$$b' = p_{21}a + p_{22}b + p_{23}c$$
$$c' = p_{31}a + p_{32}b + p_{33}c$$

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$a' = Pa$$

$$a = q_{11}a' + q_{12}b' + q_{13}c'$$
$$b = q_{21}a' + q_{22}b' + q_{23}c'$$
$$c = q_{31}a' + q_{32}b' + q_{33}c'$$

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix} \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix}$$

$$a = Qa' \qquad PQ = I$$

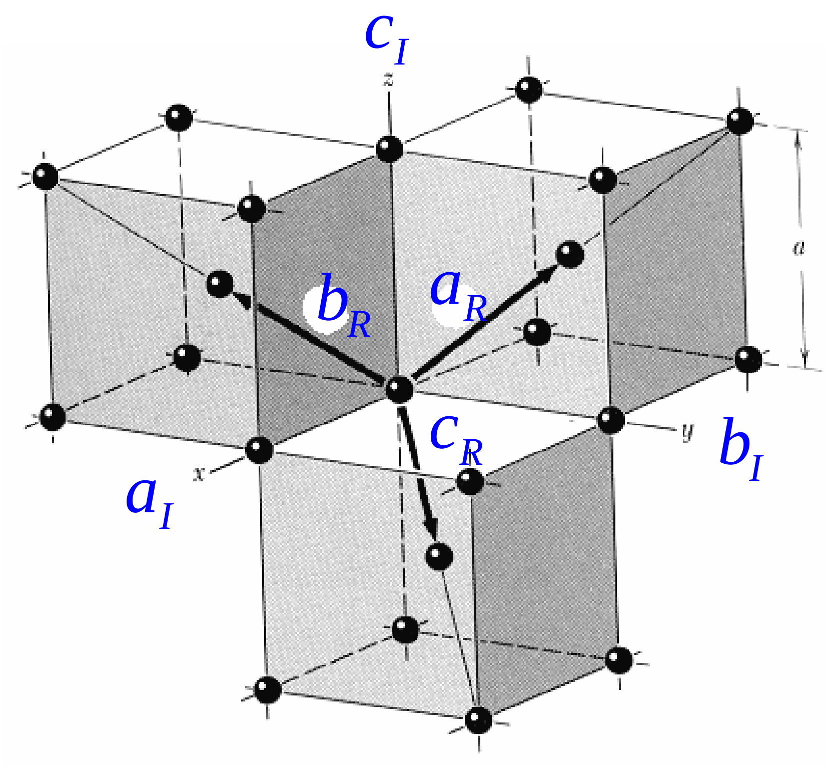
Transformation of Coordinate System

– bcc to rhombohedral

$$a_R = -\frac{1}{2}a_I + \frac{1}{2}b_I + \frac{1}{2}c_I$$

$$b_R = \frac{1}{2}a_I - \frac{1}{2}b_I + \frac{1}{2}c_I$$

$$c_R = \frac{1}{2}a_I + \frac{1}{2}b_I - \frac{1}{2}c_I$$



$$a_I = 0a_R + 1b_R + 1c_R$$

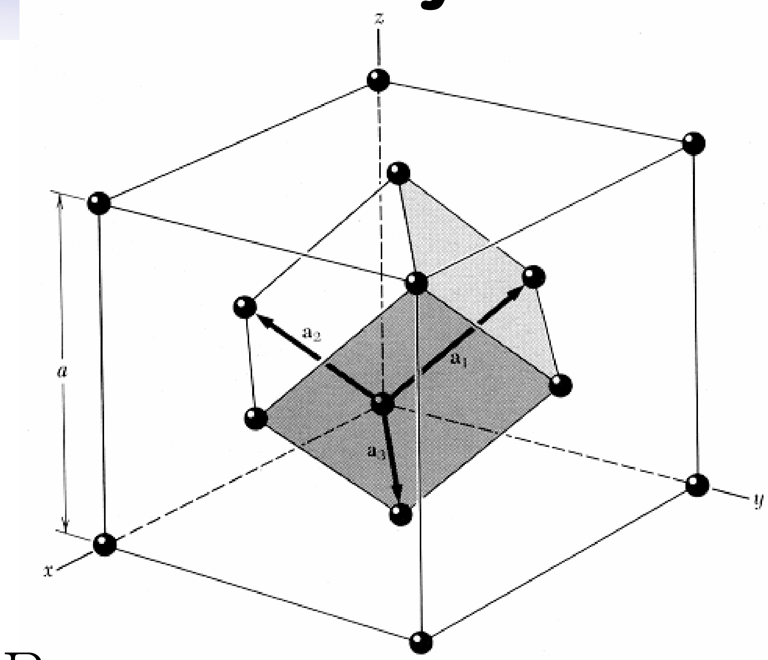
$$b_I = 1a_R + 0b_R + 1c_R$$

$$c_I = 1a_R + 1b_R + 0c_R$$

$$P = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \qquad Q = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Transformation of Coordinate System

- fcc to rhombohedral



- trigonal R-rhombohedral P