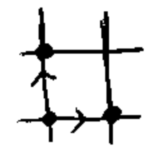
Lect 4 Crystal lattice (Chap 4 Ashcroft & Mermin)

§ Bravais lattice and primitive vectors

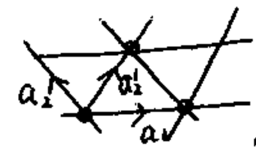
discrete translation symmetry : $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

where $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are linearly independent, (n_1, n_2, n_3) are integers.
but not necessarily orthogonal



example 2D : square $\vec{R} = n_1 \hat{x} + n_2 \hat{y}$

triangular $\vec{R} = n_1 \hat{x} + n_2 \left(-\frac{\hat{x}}{2} + \frac{\sqrt{3}}{2} \hat{y}\right)$

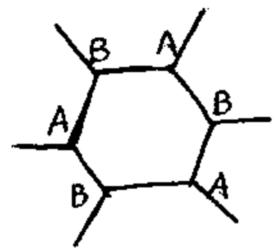


primitive vectors are not unique.

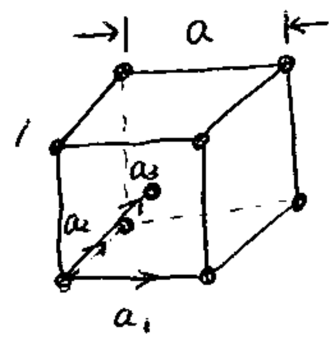
3D simple cubic $\vec{R} = n_1 \hat{x} + n_2 \hat{y} + n_3 \hat{z}$

① Honeycomb lattice is <u>not</u> Bravais lattice

points A and B cannot be related through translation. A & B can be related by rotation or reflection.



② bcc lattice



two simple cubic lattices, one is at the center points of the other.

$\vec{R} = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3$

$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$

but this set of primitive basis doesn't represent the cubic symmetry well.

Coordination number $z = 8$.

bcc is a bipartite lattice.

another better choice

$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$

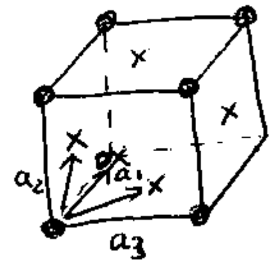
$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$

$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$

3 fcc: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$,

$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$.

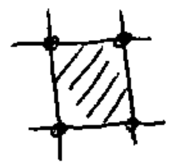
coordination number 12.



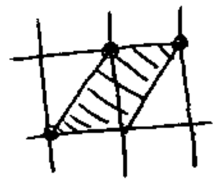
§ primitive unit cell:

A smallest volume of cell can be used by translation to pave the space.

The choice of unit cell isn't unique



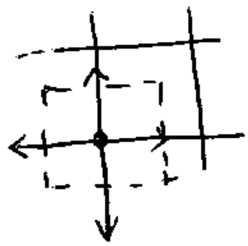
or



each unit cell only contains one lattice site of the Bravais lattice.

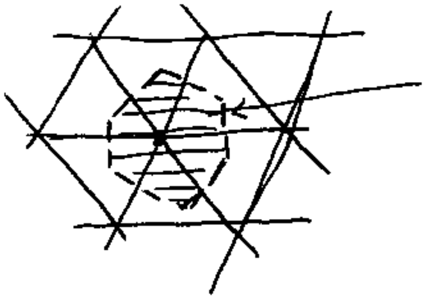
✡ Wigner-Seitz unit cell — preserve the lattice symmetry

1 square lattice



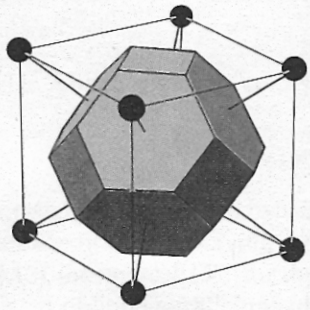
for one lattice site, draw the lattice vectors to nearest neighbors. Draw the perpendicular bisect lines, they enclose the W-S unit cell.

2 triangular lattice



six fold rotational symmetry

Figure 4.15
The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a "truncated octahedron"). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).



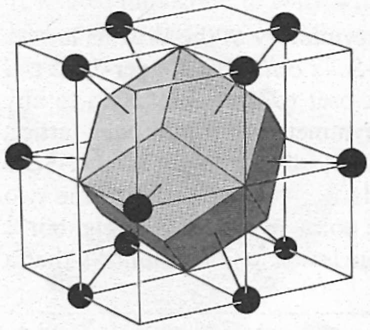
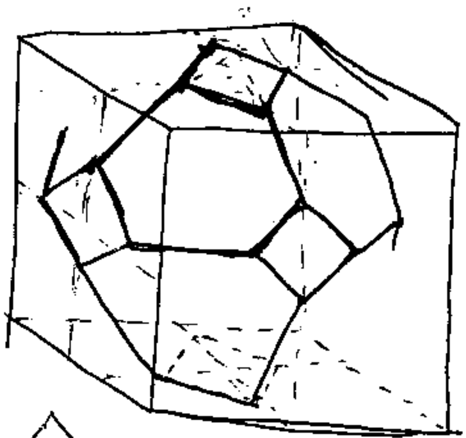


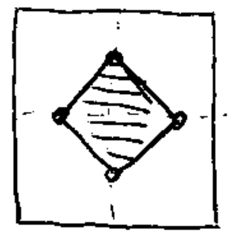
Figure 4.16
Wigner-Seitz cell for the face-centered cubic Bravais lattice (a "rhombic dodecahedron"). The surrounding cube is *not* the conventional cubic cell of Figure 4.12, but one in which lattice points are at the center of the cube and at the center of the 12 edges. Each of the 12 (congruent) faces is perpendicular to a line joining the central point to a point on the center of an edge.

③ body-centered:

truncated octahedron:



each face has a small square located as

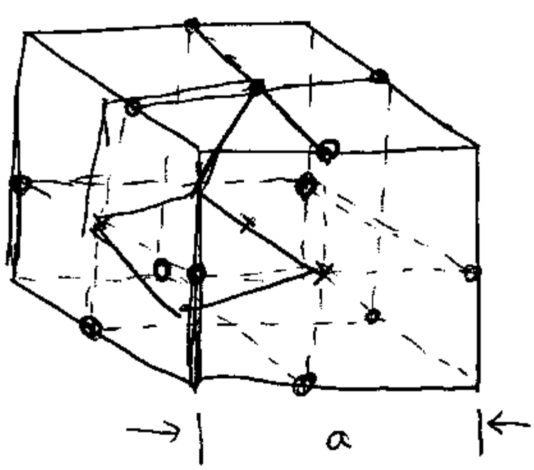


connect all the vertices.

excise: prove other 8 faces are regular hexagons.

④ fcc

rhombic dodecahedron



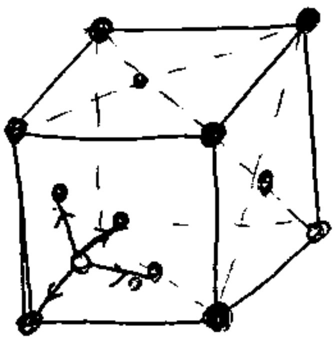
around the center, first construct a small cube with edge length $\frac{a}{2}$. Connecting the center, and four points of each face, we get a pymial, do the reflection respect that face, we get the mirror point of the center. The six mirror points, and 8 vertices of the small cube $\Rightarrow$ 14 vertices of dodecahedron

1) the 6 mirror points are actually the face centers of the big cube with edge length a.
2) The 8 vertices of the small cube are (\pm a/4, \pm a/4, \pm a/4)

Ex: prove each rhombic face has the edge length $\frac{\sqrt{3}}{4}a$. and angles $\cos^{-1}\frac{1}{3}$ and $\pi - \cos^{-1}\frac{1}{3}$.

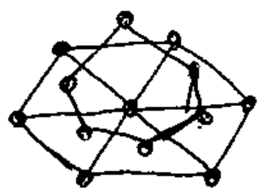
Diamond lattice:

Two interpenatrating fcc lattice with a relative displacement vector $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$



hexagonal close-pack (hcp)

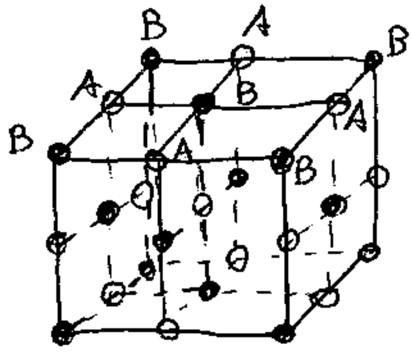
two simple hexagonal Bravais lattice with a relative displacevector $\frac{\vec{a}_1}{3}+\frac{\vec{a}_2}{3}+\frac{\vec{a}_3}{2}$



coordination number 12

Sodium-Chloride lattice

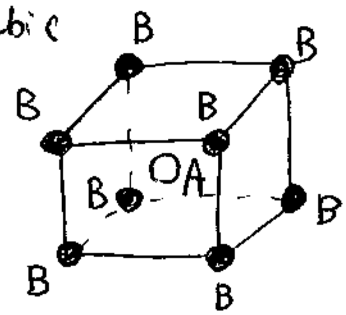
Sodium and chlorine atom alternatively occupies the sites of simple cubic lattice.



the Bravais lattic is fcc.

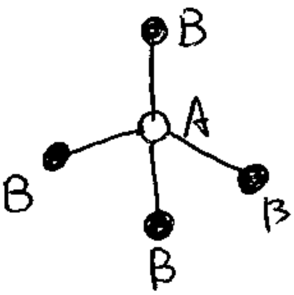
Cesium-Chloride

Ce and Cl atom alternatively occupies sites of bcc lattice The Bravais lattice is simple Cubic



Zinc-blende : ~~Dimor~~ diamond lattice (AB)

~~a~~ Bravis lattic is fcc.



no-inversion symmetry

The Reciprocal lattice

For each lattice site of Bravais lattice R_i if for a wavevector K (a) which satisfies $e^{iKR_i} = 1$, then K is a reciprocal lattice vector.

Let $\vec{a}_1, \vec{a}_2, \vec{a}_3$ as a set of basis of primitive vector, and $\vec{b}_1, \vec{b}_2, \vec{b}_3$ as a set of basis of reciprocal lattic vector.

we have $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$. we write in terms of matrix form

$$\begin{pmatrix} a_{1,x} & a_{1,y} & a_{1,z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{pmatrix} \begin{pmatrix} b_{1x} & b_{2x} & b_{3x} \\ b_{1y} & b_{2y} & b_{3y} \\ b_{1z} & b_{2z} & b_{3z} \end{pmatrix} = 2\pi I$$

$$\begin{pmatrix} b_{1x}, & b_{2x}, & b_{3x} \\ b_{1y}, & b_{2y}, & b_{3y} \\ b_{1z}, & b_{2z}, & b_{3z} \end{pmatrix} = 2\pi \begin{pmatrix} a_{1x} & a_{1y} & a_{1z} \\ a_{2x} & a_{2y} & a_{2z} \\ a_{3x} & a_{3y} & a_{3z} \end{pmatrix}^{-1} = 2\pi \frac{\begin{pmatrix} a_{2y}a_{3z} - a_{2z}a_{3y}, & \cdots, & \cdots \\ a_{2z}a_{3x} - a_{2x}a_{3z}, & \cdots, & \cdots \\ a_{2x}a_{3y} - a_{3y}a_{3z}, & \cdots, & \cdots \end{pmatrix}}{\det(a_{i,\alpha})}$$

$$= 2\pi \frac{1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \left[\vec{a}_2 \times \vec{a}_3, \ \vec{a}_3 \times \vec{a}_1, \ \vec{a}_1 \times \vec{a}_2 \right]$$

for $\vec{K} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$, $\quad \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

$$\vec{K} \cdot \vec{R} = 2\pi (m_1 n_1 + m_2 n_2 + m_3 n_3)$$

<u>The reciprocal lattice of the reciprocal lattice is the original lattice.</u>

$$\vec{b}_1 = \frac{2\pi}{\Omega} \vec{a}_2 \times \vec{a}_3$$

$$\vec{b}_2 = \frac{2\pi}{\Omega} \vec{a}_3 \times \vec{a}_1 \qquad \Omega = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

$$\vec{b}_3 = \frac{2\pi}{\Omega} \vec{a}_1 \times \vec{a}_2$$

$$\det a \cdot \det b = (2\pi)^3 \Rightarrow \vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$$

The product of volumes of the unit cells of the primitive & reciprocal lattice is $(2\pi)^3$.

Examples: ① Simple cubic lattice $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = a\hat{z}$

$\Rightarrow \vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$, $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$.

② fcc $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$, $\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$

$$\vec{a}_2\times\vec{a}_3 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}\frac{a^2}{4} = \frac{a^2}{4}\left[-\hat{x}+\hat{y}+\hat{z}\right]$$

$$\vec{a}_3\times\vec{a}_1 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix}\frac{a^2}{4} = \frac{a^2}{4}\left[\hat{x}-\hat{y}+\hat{z}\right]$$

$$\Omega = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \left(\frac{a}{2}\right)^3\cdot 2 = \frac{a^3}{4}$$

$$\vec{a}_1\times\vec{a}_2 = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix}\frac{a^2}{4} = \frac{a^2}{4}\left[\hat{x}+\hat{y}-\hat{z}\right]$$

$\Rightarrow \vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$ $\vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$, $\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

Which the basis of the bcc lattice with side length $\frac{4\pi}{a}$.

③ bcc with $\vec{a}_1 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$, $\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$

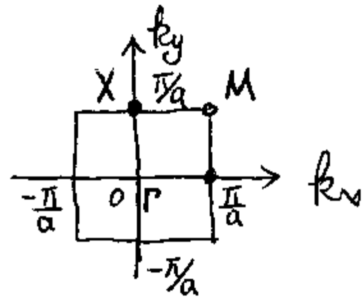
Similarly $\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z})$, $\vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$, $\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$.

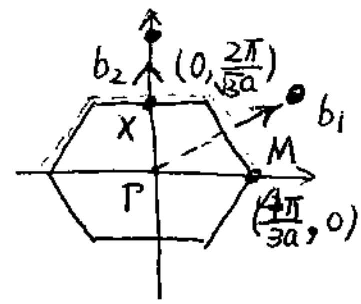
Which is the basis of fcc lattice with the side length $\frac{4\pi}{a}$.

§ First Brillouin Zone. (BZ).

The Wigner - Seitz unit cell of the reciprocal lattice is the first BZ. (FBZ)

① Square lattice





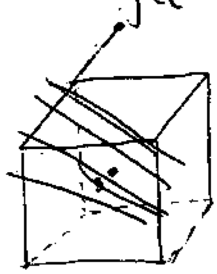
② Triangular lattice

$a_1 = a(1, 0)$, $a_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2})$

$$(b_1, b_2) = (2\pi)^2 a^{-2} \begin{bmatrix} 1 & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix}^{-1} = \frac{4\pi^2}{a^2} \frac{\begin{bmatrix} \frac{\sqrt{3}}{2} & 0 \\ \frac{1}{2} & 1 \end{bmatrix}}{\frac{\sqrt{3}}{2}} = \left(\frac{2\pi}{a}\right)^2 \begin{bmatrix} 1 & 0 \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{3}} \end{bmatrix}$$

③ FBZ of bcc lattice.

fcc lattice.



write down the coordinates of each vertex and center points of each face of the FBZs of the reciprocal lattices of bcc and fcc lattice.

Classification of Bravais lattices

§1 sysmmetry operations of a simple Bravais lattice (not dimond, honeycomb, NaCl, CsCl, Zn-Blend..)

1. Translations through Bravais lattice vectors
2. Operations that leave a particular point fixed (rotation, inversion, reflection, lattice
3. combinations of 1 and 2

all of the space operations form the space group ← group:

def: a group of operations: any combination of operations remain in the group.

group theory: early 19th century

Abel, Galois, solution of equations of n-th power ($n \geq 5$).

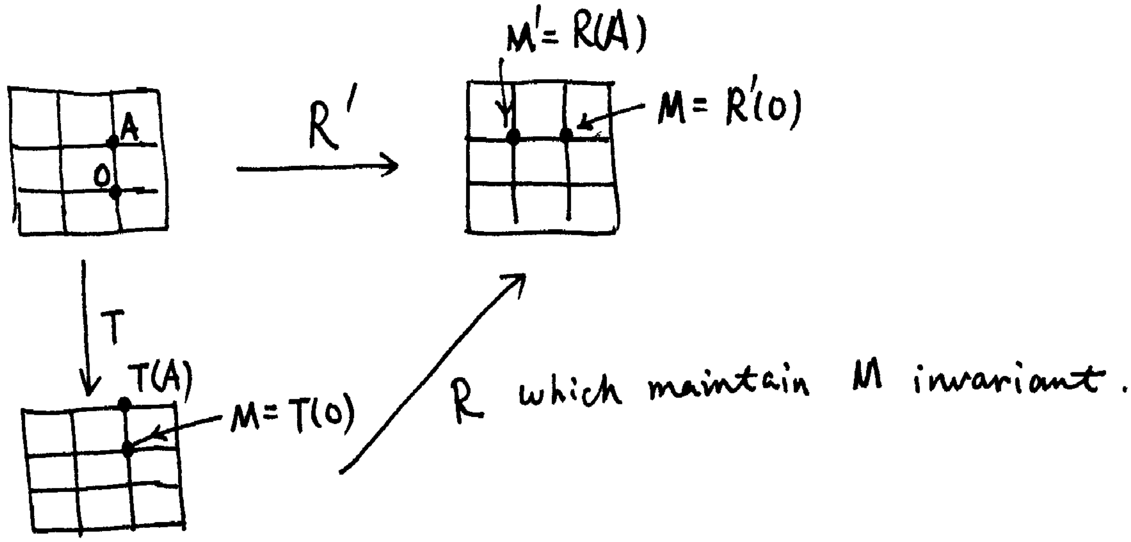
permutation group, Lie — continuous group

Weyl, Wigner, (introduce group theory to physics.

The principle of symmetry is one of the most important principles of physics.

★ there are some operations that leave the lattice invariant, but they do not leave any site fixed. R' These operations can be decomposed to combinations of translation (T) & operations with one sites fixed. (R)

To be specific, we want fix the origin O. Suppose in operation R', it transfer $O \longrightarrow \vec{M}$. Then we choose the translation of $T: O \rightarrow \vec{M}$, then the image of O at $\vec{M}$. the resulting lattice of this translation, has the same it can be performed a further operatation R, which fixes $\vec{M}$.

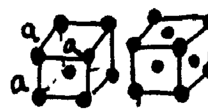


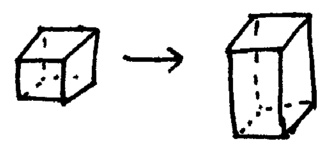
★ The set of operations in ② ⇒ $\boxed{\text{point group}}$.

§2. 7 crystal systems and 14 Bravais lattices

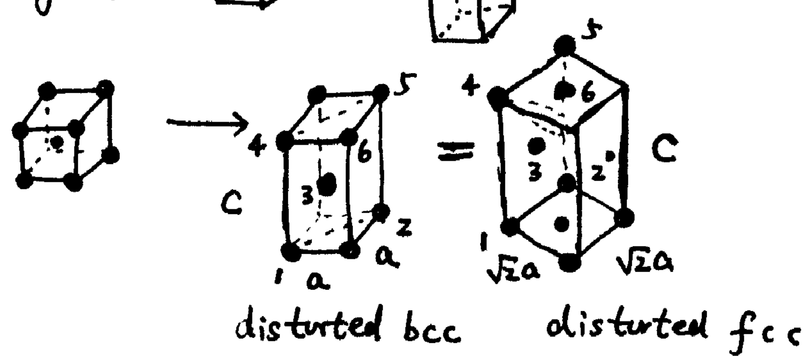
point group classification

adding different translation pattern

① Cubic : simple cubic, bcc, fcc  — 3

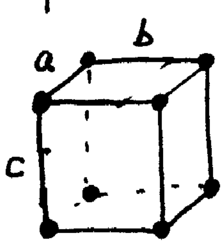
② tetragonal : a. Simple tetragonal  — 2

b. Centered tetragonal



③ Orthorhombic

a. Simple orthorhombic



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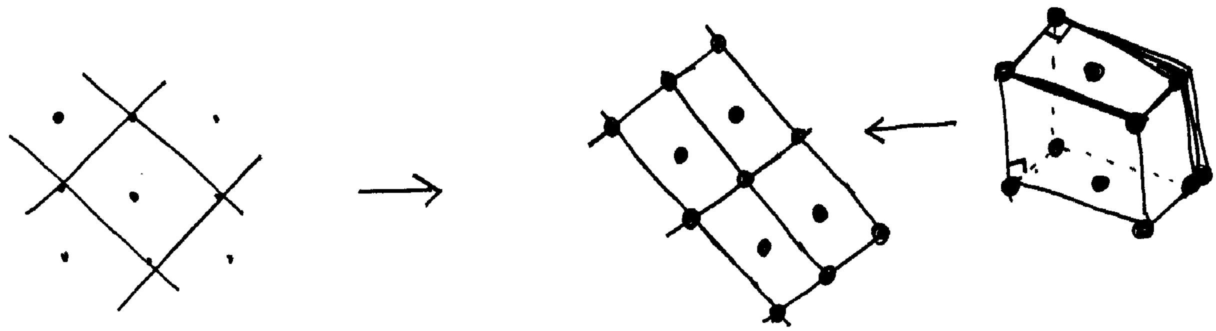
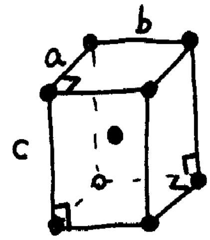
b: base-centered orthorhombic – distortion along diagonal



c. body-centered orthorhombic

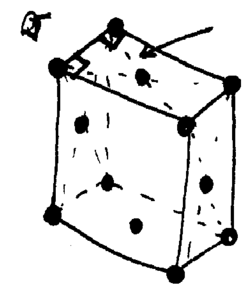


non-equivalent again

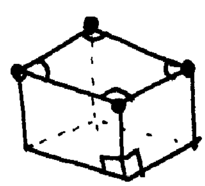
⟷

because of rectangle.
lattice ≠ square lattice

d face-centered orthorhombic

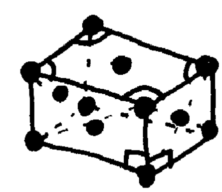


④ monoclinic : distortion of the rectangler faces perpendicular to c-axis into parallelogrames.



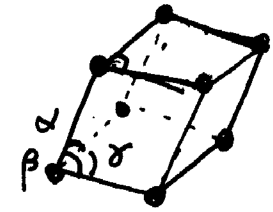
simple monoclinic

(disturd simple orth…
and base-centered orth…)



– 2

centered monoclinic orthrohombic



$\alpha \neq \beta \neq \gamma$

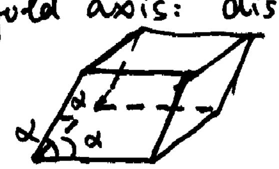
⑤ triclinic : lowest sym. only inverse

– 1

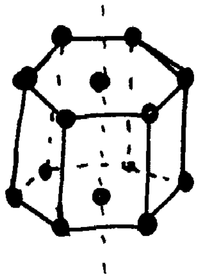
no-need to new site in the face center

⑥ triagnoal – 3-fold axis: distort cube along body diagnal

rhombohedral



7 hexagonal



(hcp is not the simple hexagnal lattice).

← hexagnoal Bravias lattice.

7- cystal systems

total:
14-
Bravais
lattice

{ Cubic (3), tetrohedral (2). orthorhumbic (4), monoclinic (2)
{ triclinic (1), triagonal (1), hexagonal (1). = 14.

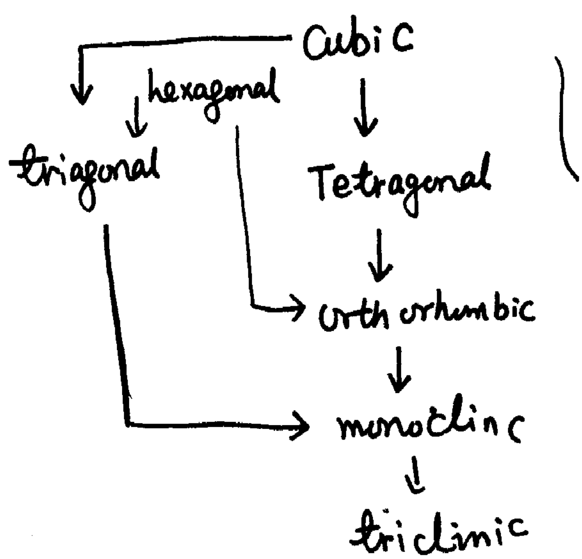
§ Cystallographic point groups

difference between Bravais lattice and cystal structure. We can put an object at each site of Bravis lattice. — cystal structure.

$\underbrace{\text{an object}}_{\text{abitary}}$

there're 32 crystallogrphic point group, but only 7 for Bravais lattice.

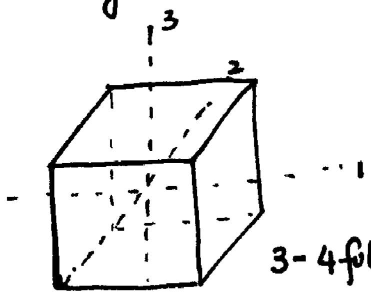
we can start from 7 Bravais lattice $\xrightarrow[\text{symmetry}]{\text{reduce}}$ other 25 cystal point group.



notations of point group:

① Cubic system : 5 different crystallographic point group.

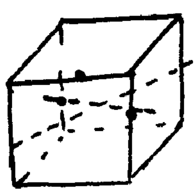
A) O_h



3-4fold axis

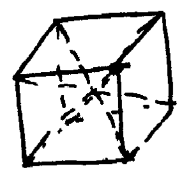
gradually breaks down the symmetry by adding internal strucutrues.

E; $R_4^1(1), R_4^1(2), R_4^1(3); R_4^3(1)\ R_4^3(2)\ R_4^3(3),\ R_4^2(1)\ R_4^2(2)\ R_4^3(2)$;



6-2foldaxis $R_2^1(1), R_2^1(2) \cdots R_2^1(6)$

4-3fold axis



$R_3^1(1)\ R_3^2(1), R_3^1(2), R_3^2(2) \cdots R_3^1(4)\ R_3^1(4)$

proper-point group operatations det $R = 1$, i.e. rotation 24

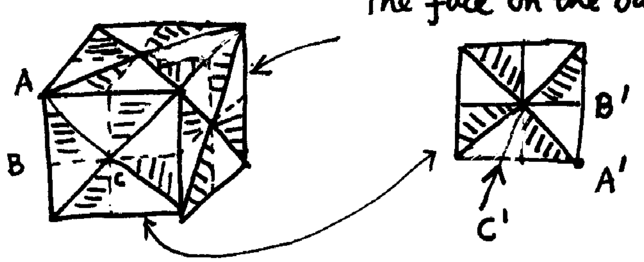
inversion ⊗ proper-point group operation 24

O_h 48 operations

I: (inversion), reflection, rotation-reflection. rotation-inversion

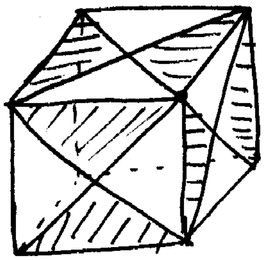
B) O: only contains proper point group operation

The face on the back



no inversion symmetry

T_h



proper operation: E, 4-fold axes → 2 fold axis

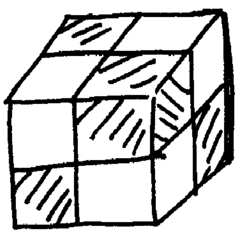
3-fold axes, 2 fold axes do not exist

$1 + 3 + 8 = 12$ } 24

Inversion ⊗ proper operation — in proper operations → 12

I, reflection, reflection-rotation, rotation-inversion

T_d

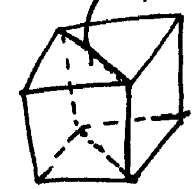


proper operation → 12 operations

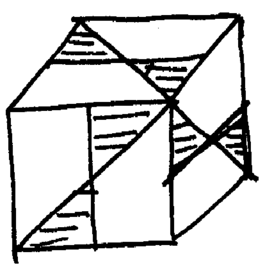
reflection planes of face-diagonal & edges

no inversion sym

reflection plane



T



only proper operation.

other point group — di hedron groups

deg

C_n: groups only contains n-fold axis $n = 2, 4, 3, 6, 1$ — +5

C_{nv}: vertice reflection plane; the plane contains the rotation axis

no C_{1v} move to C_{1h}

$n = 2, 4, 3, 6$ — +4

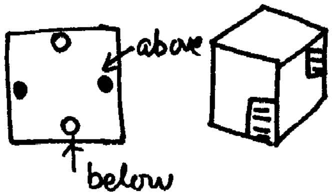
C_{nh} a mirror plane perpendicular to rotation axis

$n = 1, 2, 3, 4, 6$ — +5

no other sym. only reflection plane.

deg

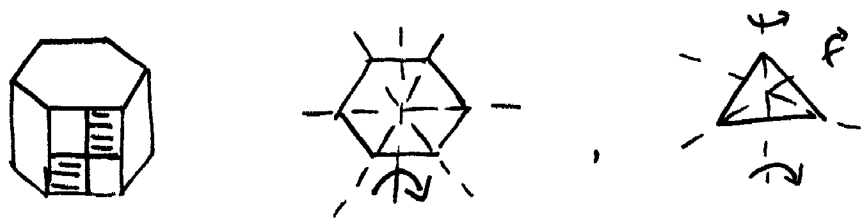
S_n: n-fold rotation-reflection axis, n-must be even



E, $\sigma_h R_n^1$, R_n^2, $\cdots$ $\rightarrow S_2$ S_4, S_6 +3

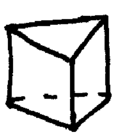
D_n 2-fold axis perpendicular to the C_n axis. $n = 2, 3, 4. 6$

+4

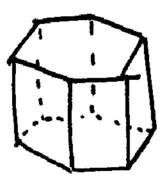


D_{nh}: D_n + mirror plane horizontal D_{2h}, D_{3h}, D_{4h} D_{6h}

D_{nh}: also contains vertical reflection planes. n: even ← inversion included
n: odd ← no inversion



D_{3h}

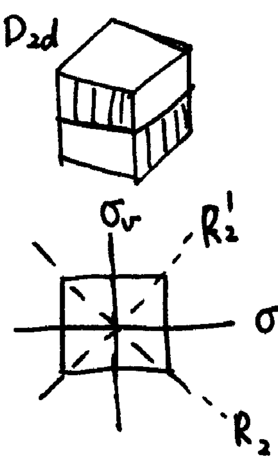


D_{6h}

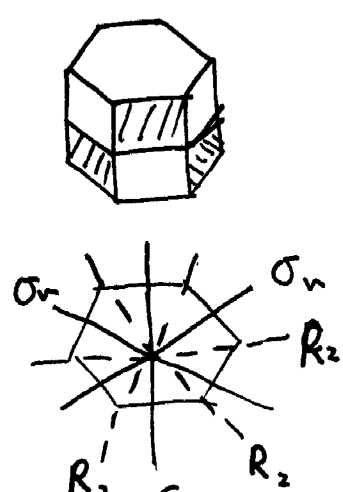
+4

D_{nd}: D_n + vertical mirror planes ~~(half of vertical planes)~~, that bisects the 2-fold axis.

D_{2d}



D_{3d}



+2

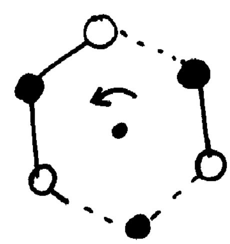
§ Space group 230

① Screw axes: translation of a vector not in the Bravais lattice followed by a rotation around the axis defined by the translation.

② glide planes: translation of a vector not in the Bravais lattice followed by a reflect plane containing that vector

ex: hcp. ① tranlation along c-axis, half a lattice const + rotation 30°

② translation along c-axis half a lattice const + reflection



A plane

shift along c-axis by $\frac{c}{2}$

B plane