北京航空航天大學
BEIHANG UNIVERSITY

Introduction to Solid State Physics

固体物理学

物理学院 李伟

Office: Room C812, Main Building of North Campus

Tel：82313568

Email：w.li@buaa.edu.cn

Wechat: Qspace-Tensor

Chapter 1 Crystal Structure

1.1 Periodic Crystal Structures

- ✓ The existence of a periodic structure lies at the heart of modern solid state physics.
- ✓ Main distinction to liquids/amorphous solids.

1.2 Fundamental Types of Lattices

1.3 Symmetry and Classifications of Bravais Lattices

1.1 Periodic Crystal Structures

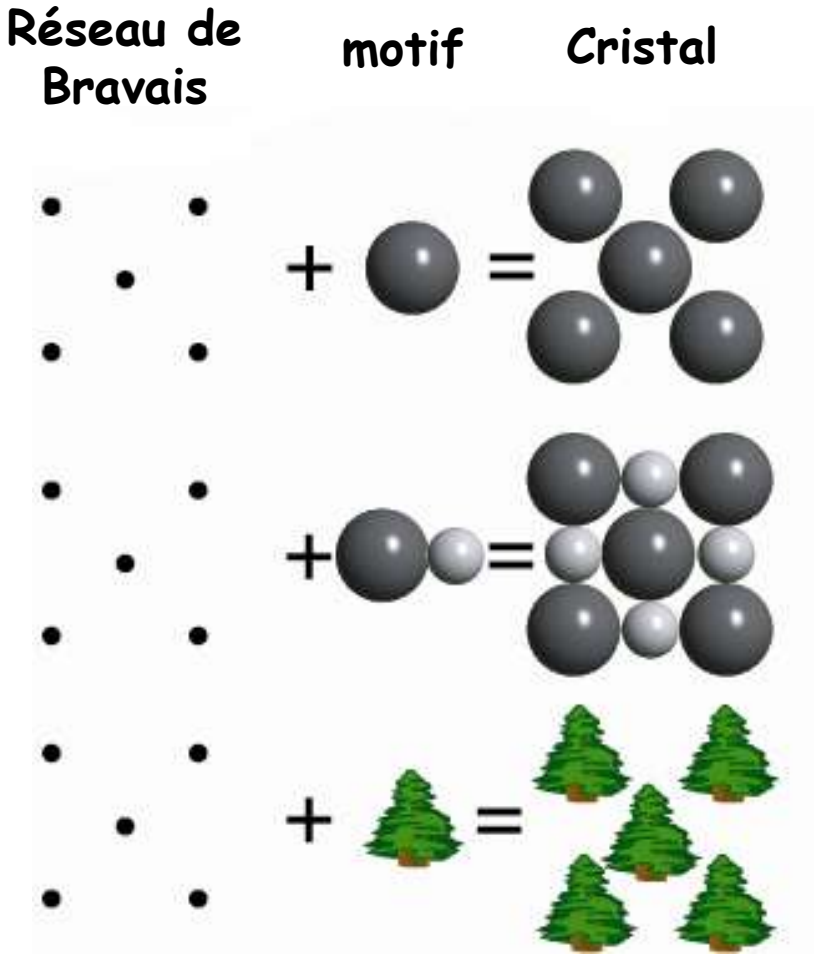
A perfectly periodic crystal?

The amethyst

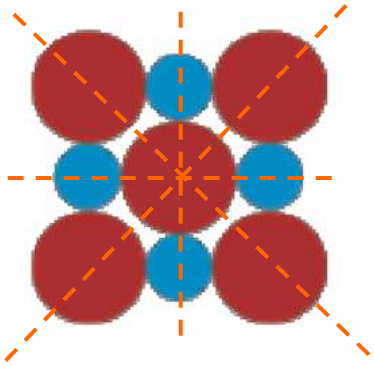
ironstone

«crystal» made out of glass

Crystal = Bravais lattice + motif/basis



The crystal can also be described by its additional symmetries



Symmetry mirror relative to 4 axes

No additional symmetry

The ideal crystal

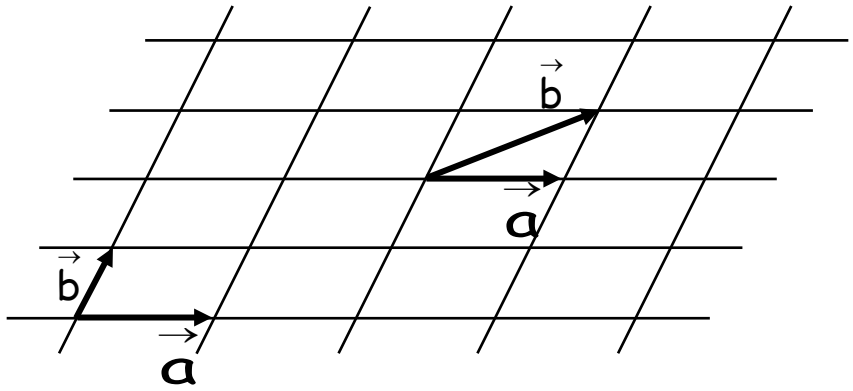
Cristal ideal = infinite repetition of identical basic structures

Cristal = Bravais lattice + Motif (basis) ⟺ translational symmetry

Bravais lattice:

In each point of the Bravais lattice, we see the crystal identically to itself in chemical composition, structure and orientation

2D: $\vec{R} = n\vec{a} + m\vec{b}$ 3D: $\vec{R} = n\vec{a} + m\vec{b} + p\vec{c}$



思考1:

布拉维格子的定义

定义1：布拉维格子是离散点按照特定的规则无穷排列组成的，从任意点看出去，晶格看起来是一模一样的（空间位置和指向）。

定义2：选定布拉维格子中的某个参考点为原点，其他任意格点都可以用下面的公式表述（且不产生多余的格点）。

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

请证明，上述两个定义是等价的。

两维布拉维格子的分类

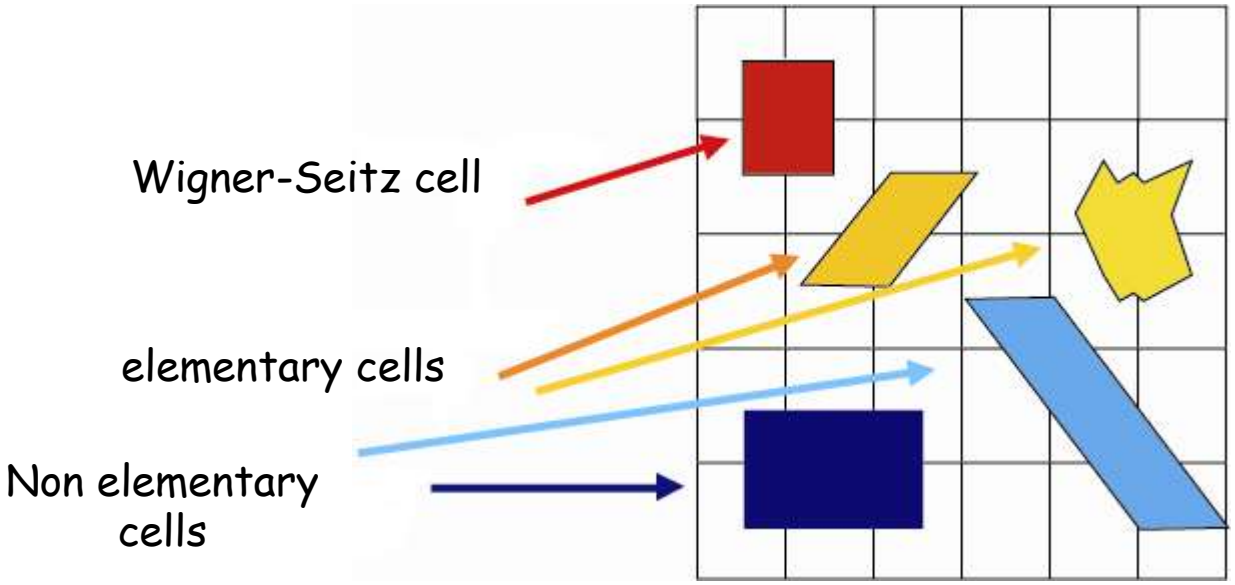
思考2:

六角格子是布拉维格子吗？是的话给出证明，不是的话按照布拉维格子+基元的方式找出其对应的布拉维格子。

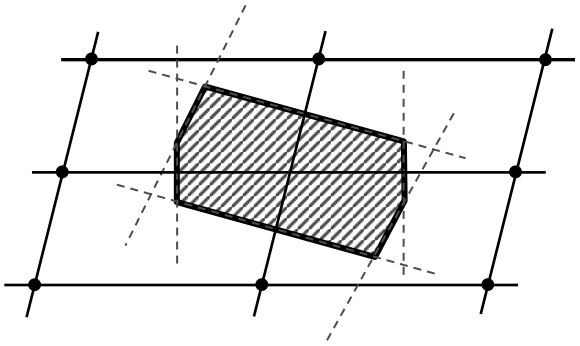
思考3:

请画出一些两维布拉维格子，并按照对称性找出两维布拉维格子的所有分类。

Bravais lattice and primitive cell



Primitive cell = the volume of space that translate to any point of the Bravais lattice completely fills the space without overlapping

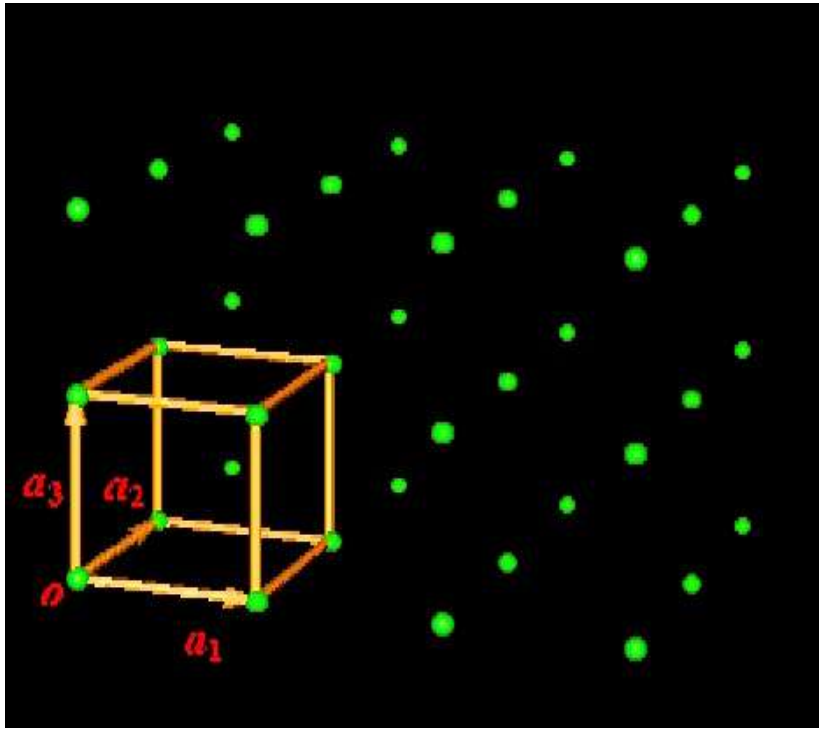


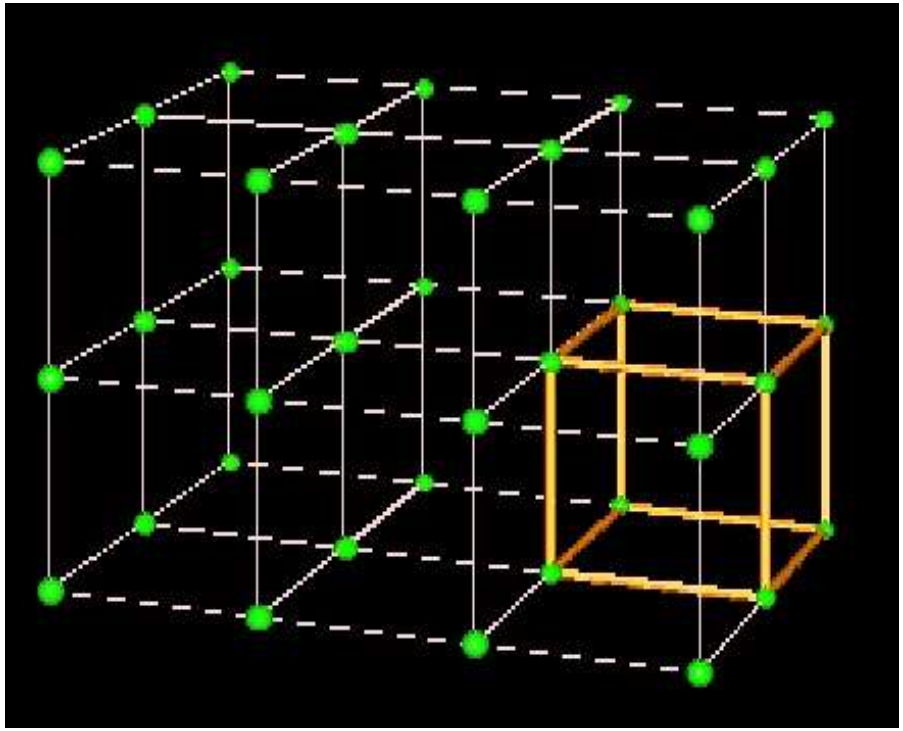
Wigner-Seitz Cell

reflecting the network of symmetry

（1）simple cubic, sc

$$\vec{a}_1 = a\hat{x} \quad \vec{a}_2 = a\hat{y} \quad \vec{a}_3 = a\hat{z}$$



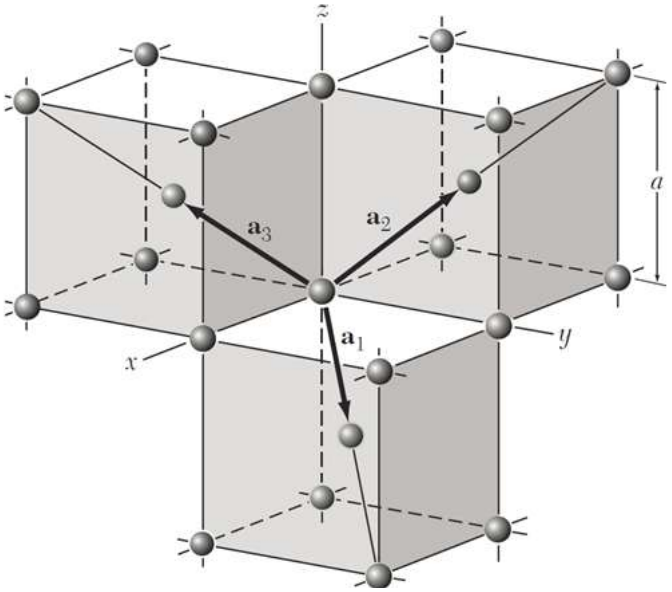


(2) body-centered cubic, bcc

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

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

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

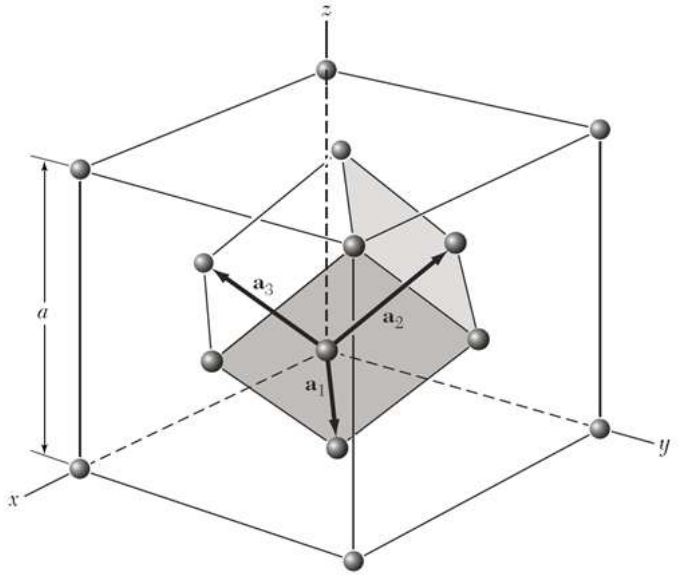


(3) face-centered cubic, fcc

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

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

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

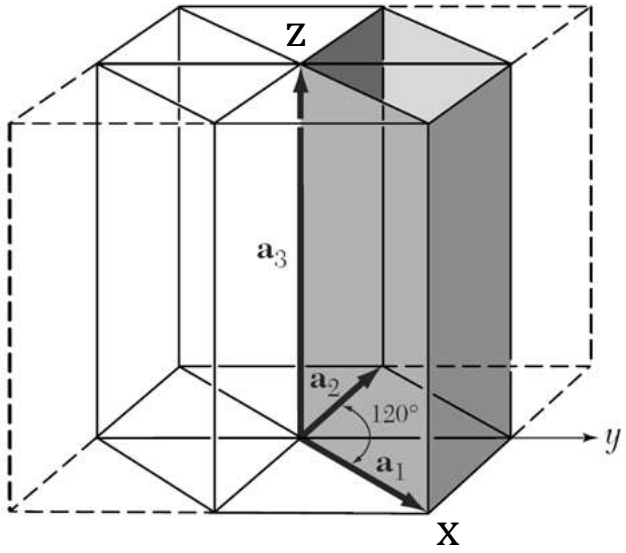


(4) simple hexagonal, sh

$$\vec{a}_1 = a\hat{x}$$

$$\vec{a}_2 = -\frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$$

$$\vec{a}_3 = c\hat{z}$$



Crystal Array & Crystal Plane

1. crystal array: The direction of a line consists of atoms/bases in a crystal.

Position vector of any lattice point on the crystall array through the origin:

$$\vec{R} = l_1'\vec{a}_1 + l_2'\vec{a}_2 + l_3'\vec{a}_3$$

$$l_1 : l_2 : l_3 = l_1' : l_2' : l_3' \Rightarrow [l_1 l_2 l_3]$$ ——index of crystal array

< > ——equivalent crystal arrays

2. Index of crystal plane: labelling the direction of crystal plane

$$h_1 : h_2 : h_3 = \frac{1}{r} : \frac{1}{s} : \frac{1}{t} \Rightarrow (h_1 h_2 h_3)$$

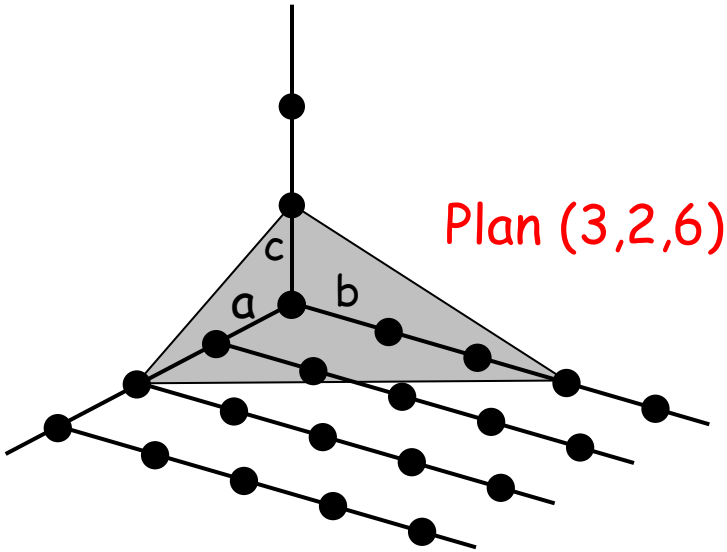
——index of crystal plane

Miller indices use the primitive vectors $\vec{a},\vec{b},\vec{c}$ consisting the convential unit cell.

{ }-- equivalent crystall planes

***A family of lattice planes*: a set of parallel, equally spaced lattice planes (with distance $d_{h_1h_2h_3}$) , which together contain all the points of the 3D Bravais lattice.**

Crystal planes: Miller indices



- Considering the intersections of the plan with 3 axes

  Intersection on ma, nb, pc **2a, 3b, 1c**

- Taking the inverse numbers m, n p

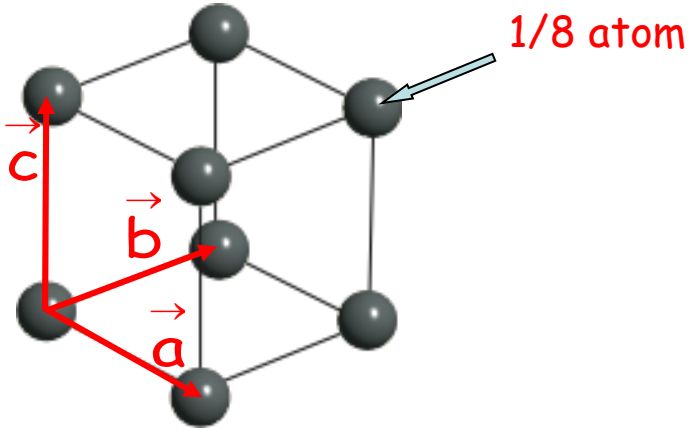
  h' = 1/m, k' = 1/n, l'= 1/p **h' = 1/2, k' = 1/3, l' = 1**

- We take the triple of the smallest integers that are in the same ratio as h', k', l'.

  h = rh', k = rk', l = rl' **h = 3, k = 2, l = 6**

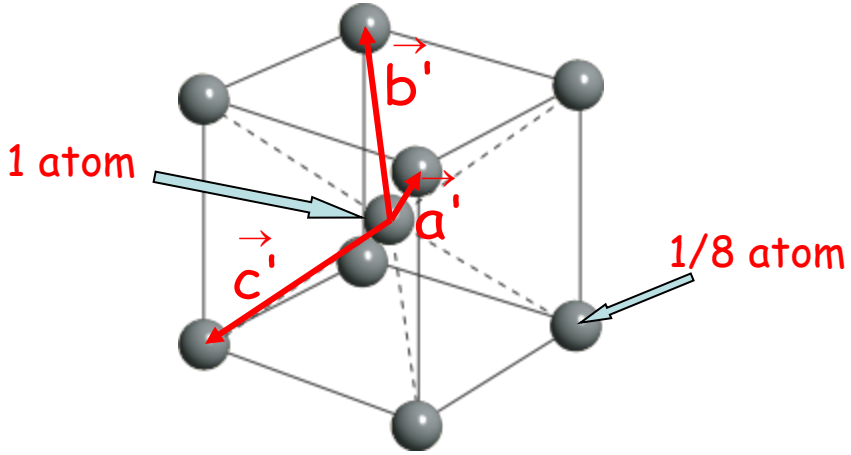
1.2 Fundamental Types of Lattices

1.2 Fundamental Types of Lattices



Simple cubic, SC

- Cubic structure = Bravais Network.
- **1 atom per unit cell.**
- 6 carbon nearest neighbors.
- Filling rate of 52%
  (model of hard spheres in contact)
- 2 cs elements crystallize in the structure:
  F and O



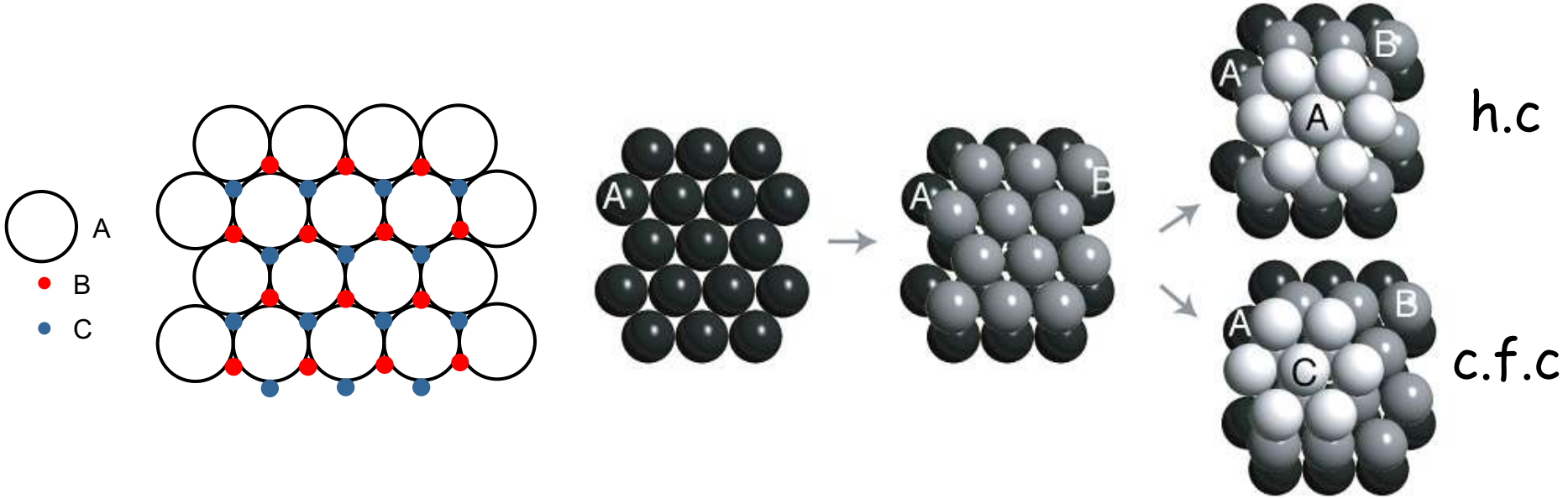
Body centered cubic, BCC

- Centered cubic structure = Bravais Network, but the cube is not a primitive cell
- **2 atoms per unit cell..**
- 8 carbon nearest neighbors.
- Filling rate of 68%.
- Exemples: W, Mo, Ta

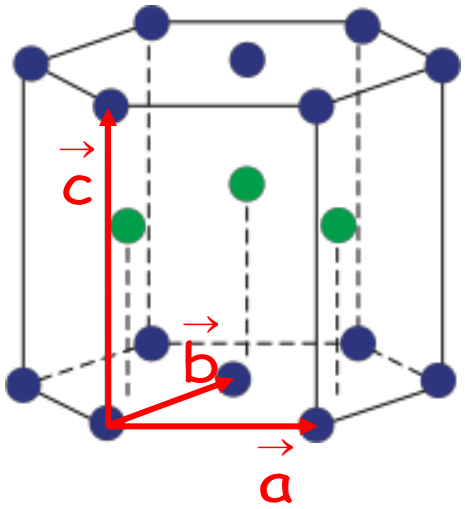
1.2 Fundamental Types of Lattices

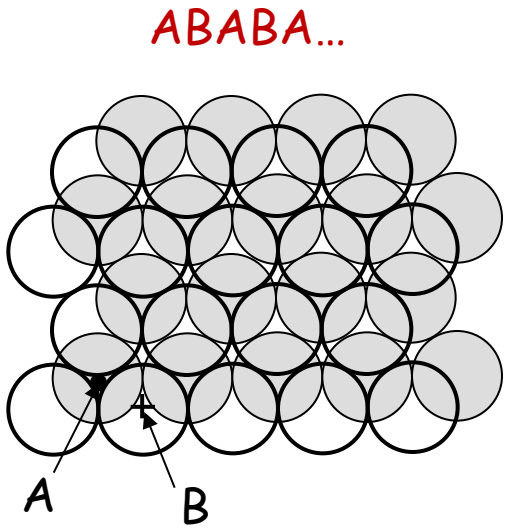
Many elements crystallize in compact crystal structures.

Crystal structures encountered particularly in molecular and metallic crystals
(spherical symmetry of the electron cloud of each atom)



Compact hexagonal Structure (h.c.p.)





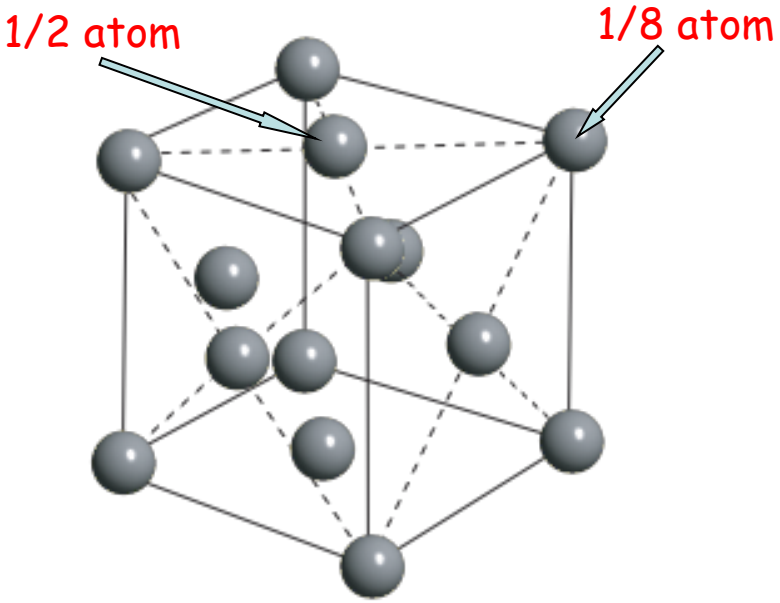
Q: Is it a Bravais lattice?

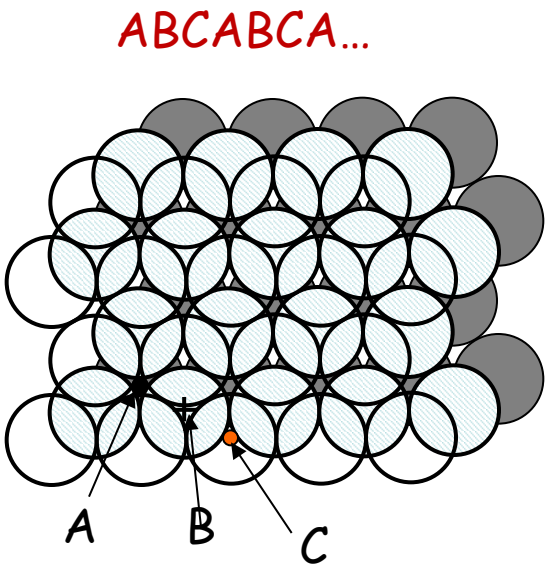
No, two interpenetrating hexagonal Bravais lattices.

What about FCC?

- **2 atom per unit cell.**
- 12 carbon nearest neighbors.
- Filling rate of 74%.

Face-centered cubic structure (fcc)

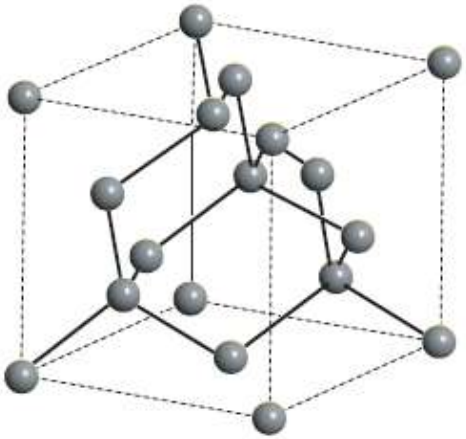


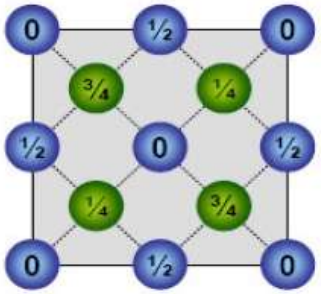


- The face-centered cubic structure is a Bravais lattice.
- **4 atoms per unit cell**.
- 12 carbon nearest neighbors.
- Filling rate of 74%

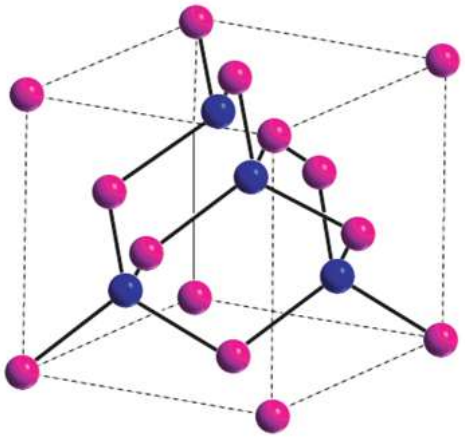
Crystal structures: diamond and zinc-blende

Structure diamond





Structure Zinc-Blende



Examples:

Exemples:

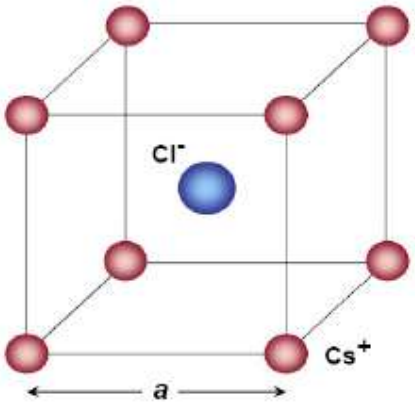
C (diamant)	a =3,57 Å
Si	a = 5,43 Å
Ge	a = 5,66 Å

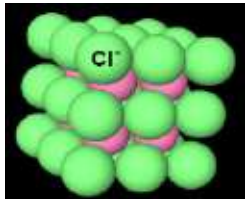
GaAs	a = 5,65 Å
InAs	a = 6,04 Å
SiC	a = 4,35 Å

Noncompact crystal structures encountered in particular in crystals covalent where the directivity of the link is important

Examples of ionic crystals

Structure CsCl

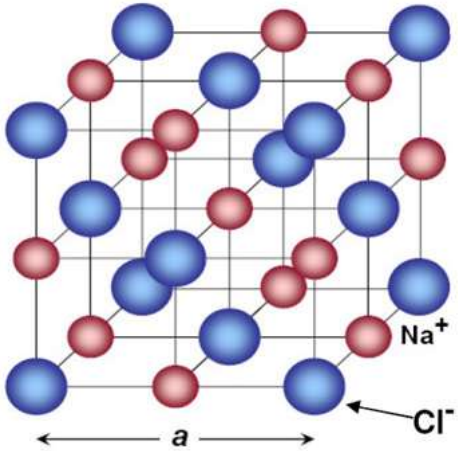


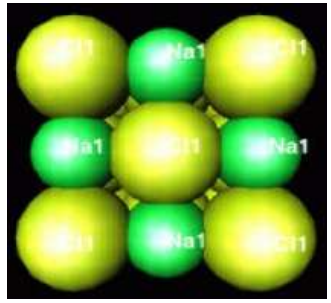


Examples:

Cu Pd	a = 2,99 Å
Cs Cl	a = 4,11Å
Cs Br	a = 4,29 Å

Structure NaCl





Examples:

Mg O	a = 4,20 Å
Na Cl	a = 5,63 Å
K Cl	a = 6,29 Å

Compactness of the structure also depends on the intensity of the electrostatic interaction, and the relative size of the ions

1.3 Classification of Bravais Lattices

I. Symmetry Elements

Few solid state physicist need to master the whole analysis of crystallography ☺

Tanslation symmetry + Rigid Operations

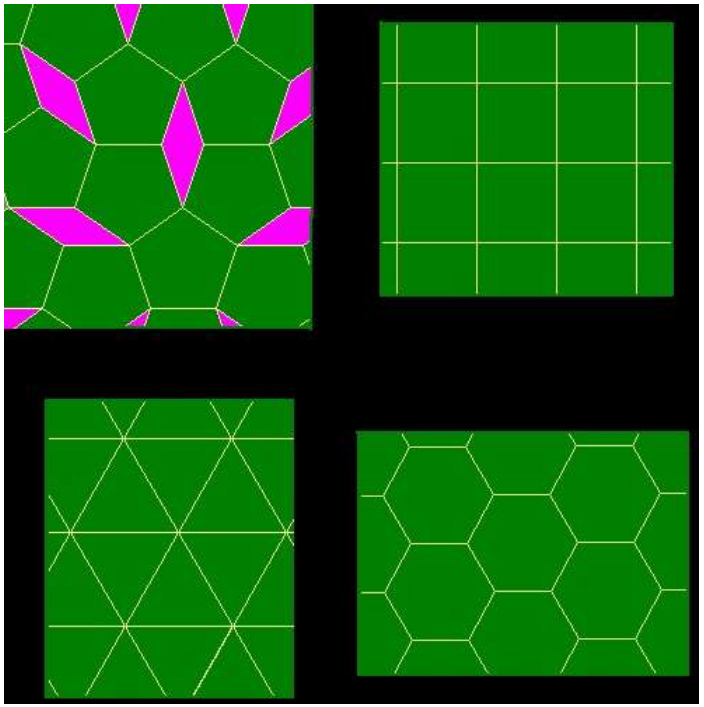
1. Inversion Symmetry:

$\vec{r} \Rightarrow \vec{r} = -\vec{r}$ **through a lattice point transform the lattice into itself, denoted as *i*.**

2. Rotation Symmetry:

Rotate the crystal about an axis $\frac{2\pi}{n}$ and take the lattice into itself. It is called n-*th* axis, denoted as C_n.

The lattice site can be considered as hard spherical ball which do not affect symmetry.



Theorem: The allowed rotational axes can only be 1st, 2nd, 3rd, 4th, and 6th axes.

$$n = 1, 2, 3, 4, 6$$

3. Reflection Symmetry:

The crystal is invariant after a reflection across a plane, denoted as $\sigma\left(m\right)$.

五次对称轴

思考4:

为何五次对称轴不出现？是否与晶格对称性不兼容？

1.3 Classification of Bravais Lattices

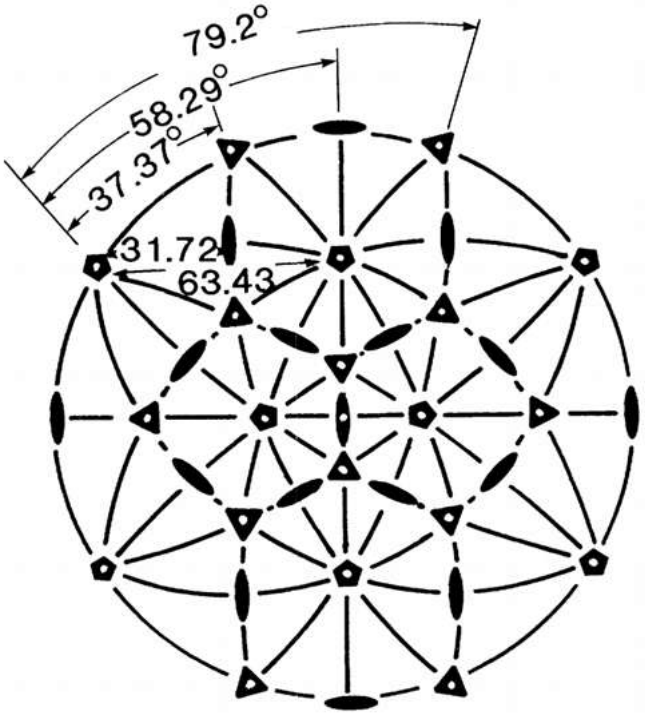
VOLUME 53, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 1984

Metallic Phase with Long-Range Orientational Order and No Translational Symmetry

D. Shechtman and I. Blech
Department of Materials Engineering, Israel Institute of Technology–Technion, 3200 Haifa, Israel

and

D. Gratias



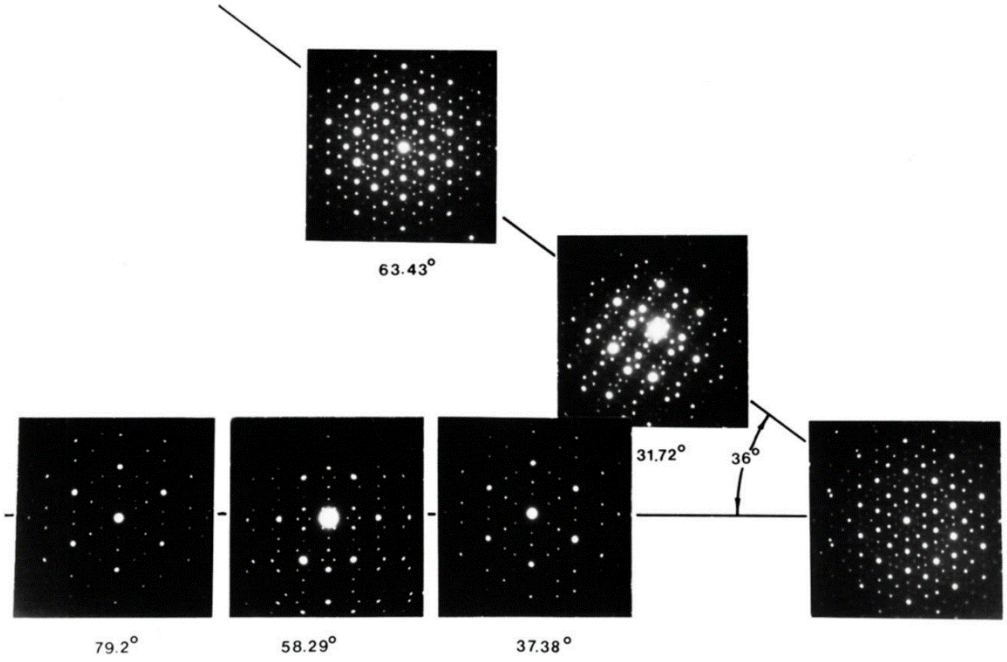


FIG. 2. Selected-area electron diffraction patterns taken from a single grain of the icosahedral phase. Rotations match those in Fig. 1.

II. Elementary symmetry operation

1. $i, C_n, \sigma(m)$
2. ***n-th*** **inversion symmetry**

Rotate along the *axis by* $\frac{2\pi}{n}$ **and then take inversion** $\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$

Therefore, in total there exists

$1, 2, 3, 4, 6, \bar{4}, i, m$ ***eight*** **independent symmetry operations**

+ translation through Bravais lattice vectors.

III. Point Group and Space Group

The full symmetry group of a Bravais lattice contains only operations of the following form:

1. Translation through Bravais lattice vectors.

2. Operations that leave a particular point of the lattice fixed.

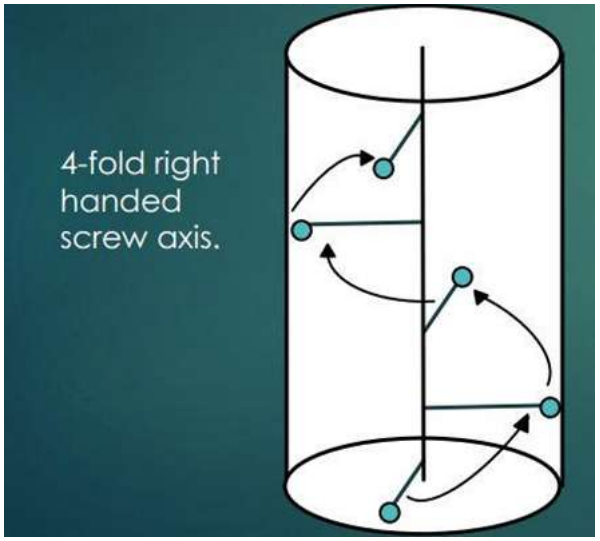
3. Successive applications of the operators of type (1) and (2).

- ✓ **Operations of type (2) form the point group**
- ✓ **23 point groups (but Bravais lattices can have 7 out of them).**
- ✓ **Add translation operations, 230 space groups.**

3. Screw Axis

rotation + translation

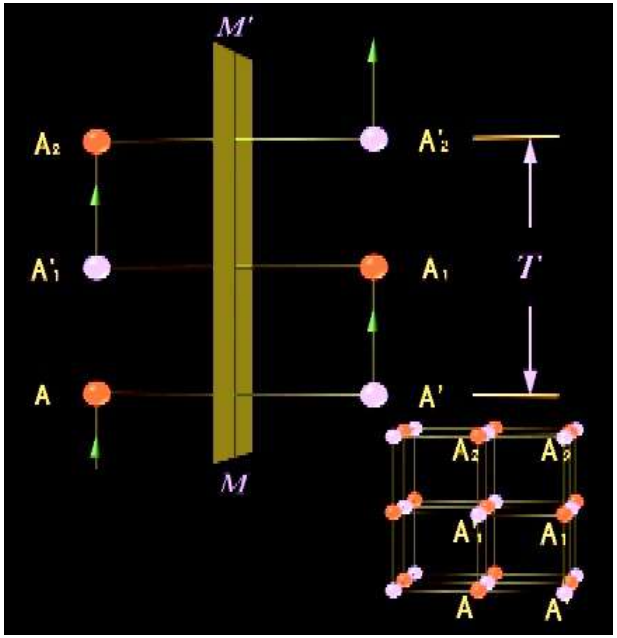
Rotate $2\pi/n$ around *u* axis, and translate *l* times of *T/n*, the crystal restores its original status.



4. Glide Plane

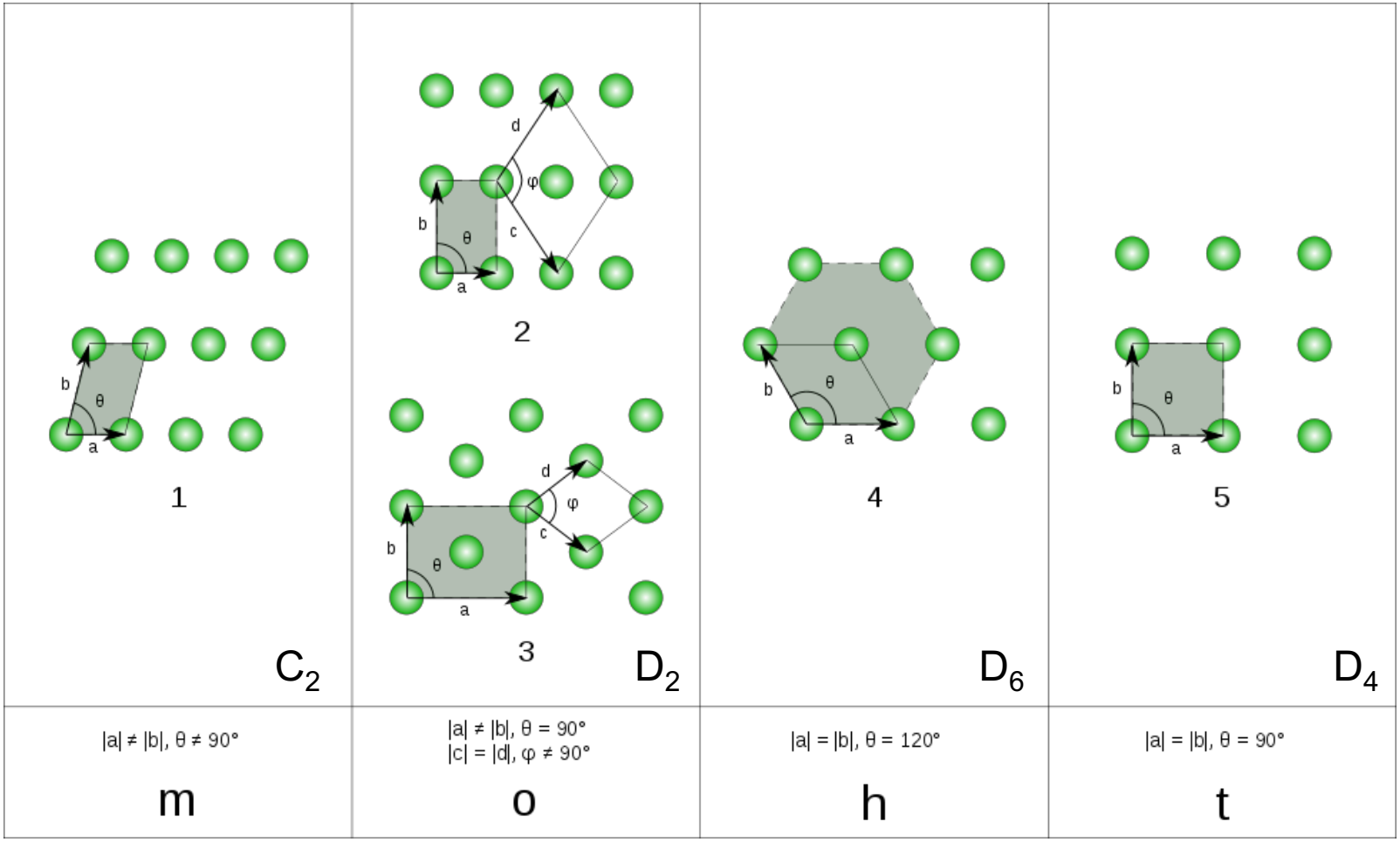
reflection + translation

Reflect across a plane, and then translate along some direction of distance *T/n*.



1.3 Classification of Bravais Lattices

Bravais lattices in 2 dimensions



In two-dimensional space, there are ***5*** Bravais lattices, grouped into ***4*** crystal families (of the same point group).

IV. 7 Crystal Systems and 14 Bravais Lattices

Table 1 The 14 lattice types in three dimensions

System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$

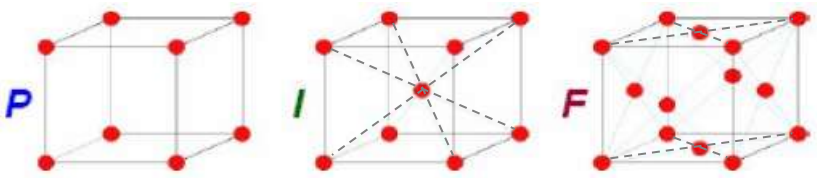
7 distinct point group and 14 distinct space group for Bravai lattice!

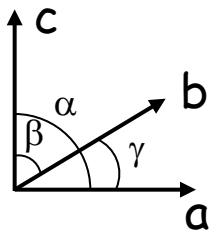
Frankenheim (1842) miscounted this number as 15;
A. Bravais is the first one get a right counting (1845).

1.3 Classification of Bravais Lattices

1. Cubic

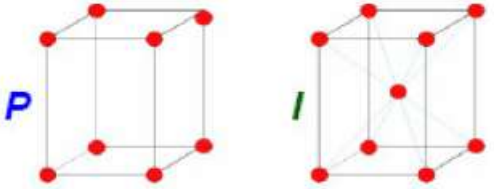
a = b = c, $\alpha = \beta = \gamma = 90^\circ$





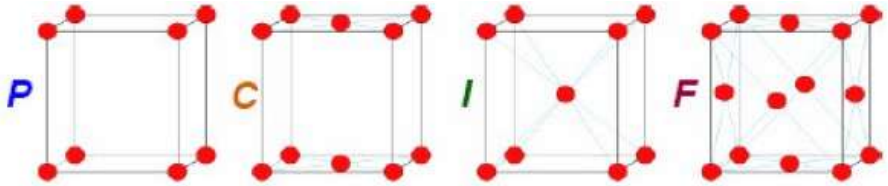
2. tetragonal

a = b ≠ c, a = b = g = 90°



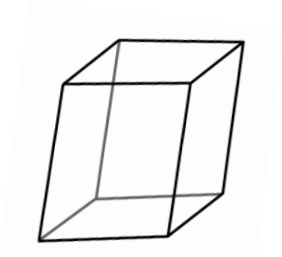
3. othorhombic

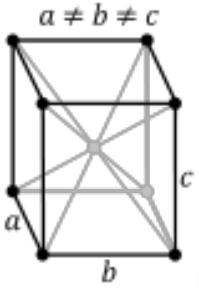
a ≠ b ≠ c, $\alpha = \beta = \gamma = 90^\circ$



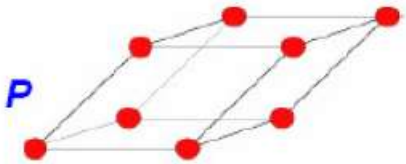
4. Monoclinic

a ≠ b ≠ c, $\alpha = \gamma = 90^\circ \neq \beta$



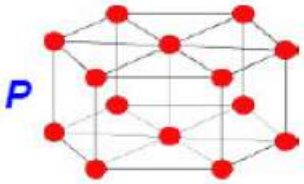


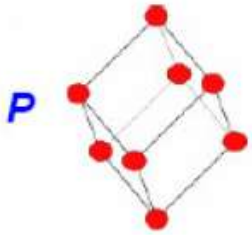
5. Triclinic a≠ b ≠ c, $\alpha \neq \beta \neq \gamma$



7. Hexagonal

a = b ≠ c, $\alpha = \beta = \gamma = 90^\circ$





6. Trigonal

a = b = c, $\alpha = \beta = \gamma \neq 90^\circ$

面心四角？

思考5:

- ✓ 立方晶系中包括简单立方、面心立方、体心立方
- ✓ 四角晶系中包括简单四角、体心四角

请问是否可以把面心四角单列为一种独立的三维布拉维格子，并说明理由。

Homework: monoclinic group

1. Why there are only two monoclinic lattices?
2. Monoclinic system can also be shown as following, is it right?