



# Outline

- **Chapter 1.1**      Periodic Array of Atoms (原子的周期性排列)
- **Chapter 1.2**      Symmetry of Crystals (晶体的对称性)
- **Chapter 1.3**      Typical Crystal Structures (典型晶体结构)
- **Chapter 1.4**      Reciprocal Lattice (倒易点阵)

# Objectives



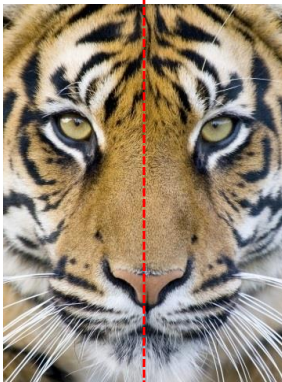
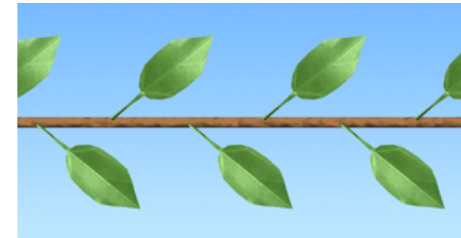
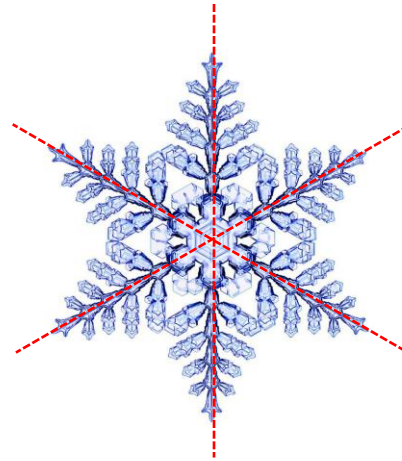
- To learn the classification of **crystal symmetries**;
- To understand the **macroscopic symmetry of crystals and its properties**;
- To learn the microscopic symmetry of crystals.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry

- ❖ Symmetry is the exact correspondence in position of parts of an object with respect to a dividing plane, line, or point.



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry of Crystals

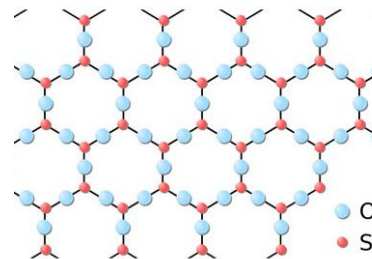
### Symmetry of Crystals

#### Macroscopic (宏观)



- ❖ Symmetry of a crystal of **finite size**.
- ❖ Focused on the **outer shape** of a crystal.
- ❖ Described by **point group**.

#### Microscopic (微观)



- ❖ Symmetry of crystal lattices of **infinite size**.
- ❖ Focused on the **inner structure** of a crystal.
- ❖ Described by **space group**.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry of Crystals

The **macroscopic symmetry** is essentially governed by the **microscopic symmetry**!

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



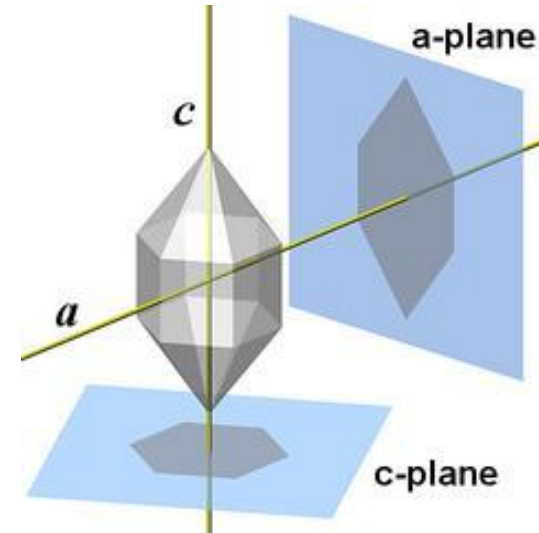
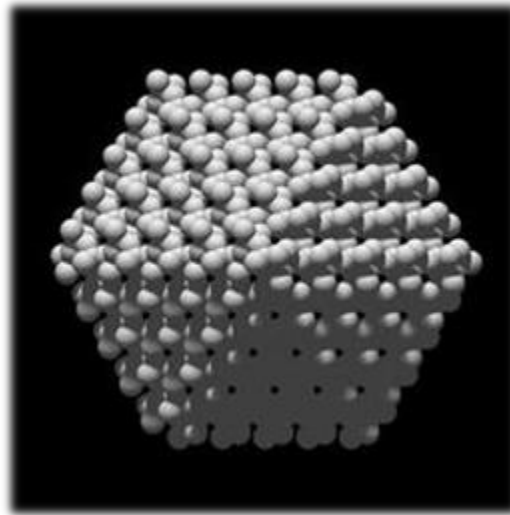
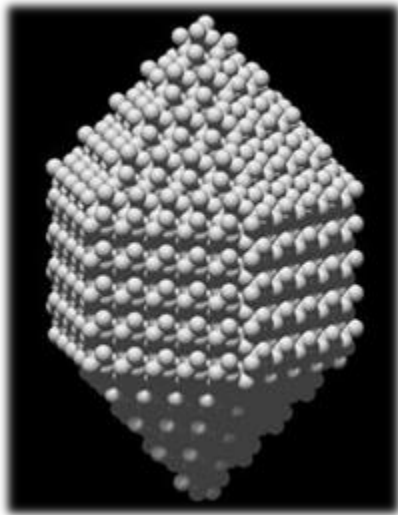
## Macroscopic Symmetry of Crystals (晶体的宏观对称性)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Macroscopic Symmetry of Crystals (晶体的宏观对称性)

- ❖ The macroscopic symmetry of crystals is the symmetry associated with the outer shape of a crystal.



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Macroscopic Symmetry of Crystals (晶体的宏观对称性)

The macroscopic symmetry of crystals can be described in terms of certain **symmetry elements** and their associated **symmetry operations**.

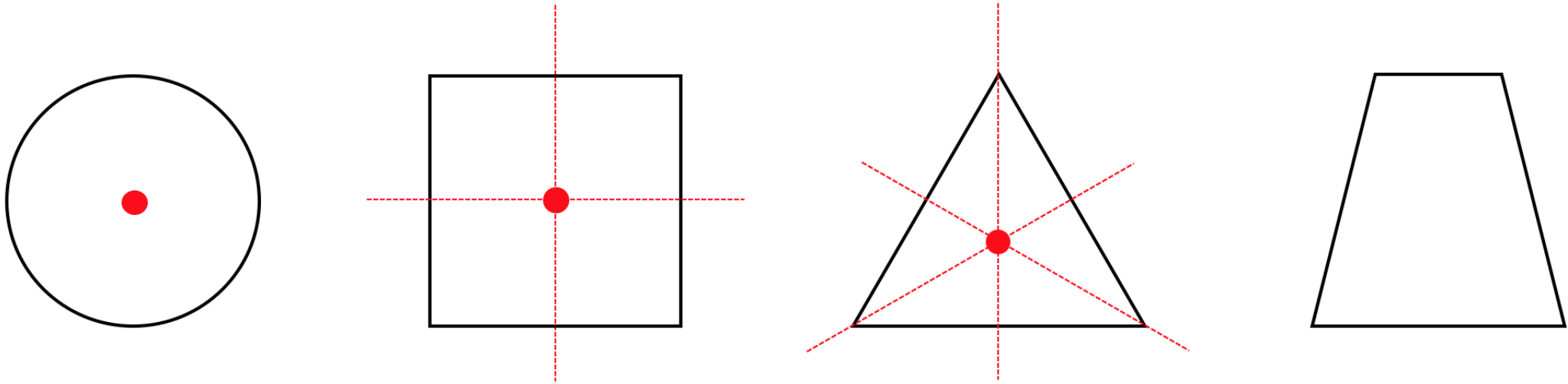


# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

- ❖ Symmetry operation is **an action of rearranging atoms** such that the crystal is transformed into a state indistinguishable from the starting state.



Examples of symmetry operation (rotation) performed to some simple geometry shapes.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

- ❖ The **physical properties** of crystals are **invariant** with respect to symmetry operations.
- ❖ Mathematically, a symmetry operation is an **orthogonal transformation** (正交变换) that keeps the crystal unchanged.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \bullet \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Coordinates  
After transformation

Coordinates  
Before Transformation

$$A_{ij} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

Orthogonal Matrix  
(正交矩阵)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

❖ The symmetry operations regarding to macroscopic symmetry include:

- 1) Identity (恒等)
- 2) Inversion (反演)
- 3) Reflection (反映)
- 4) Proper Rotation (旋转)
- 5) Improper Rotation (瑕旋转)

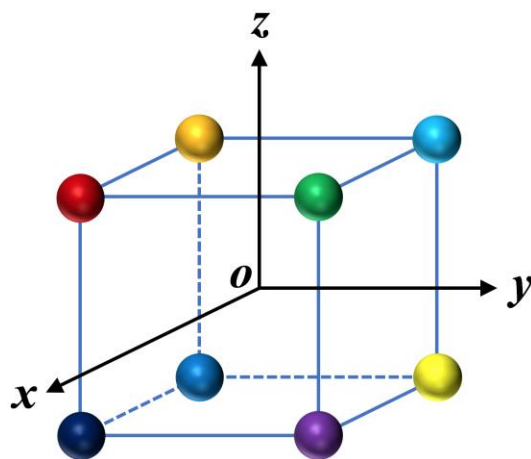
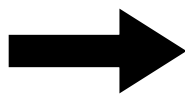
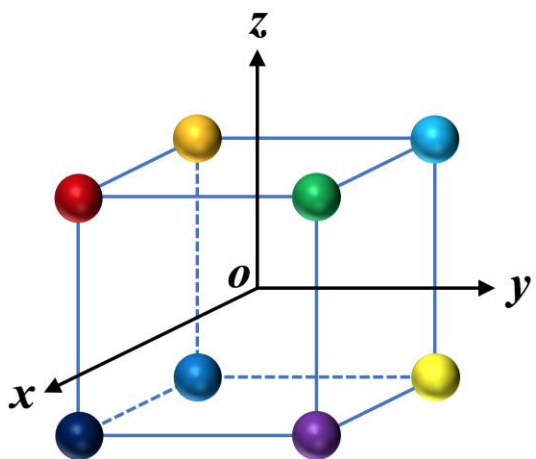
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 1) Identity (恒等)

❖ The identity operation is *doing nothing*!



$$A_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$x \quad y \quad z \quad \rightarrow \quad x \quad y \quad z$$

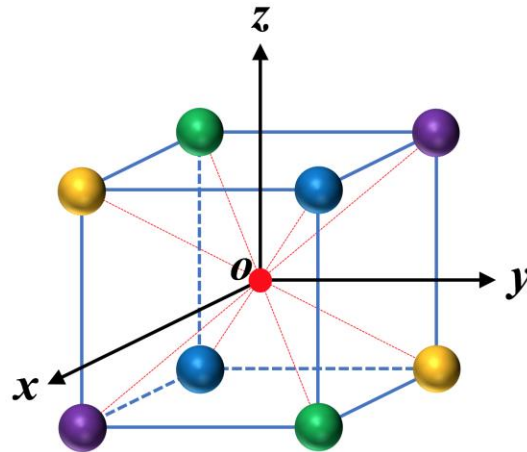
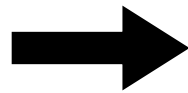
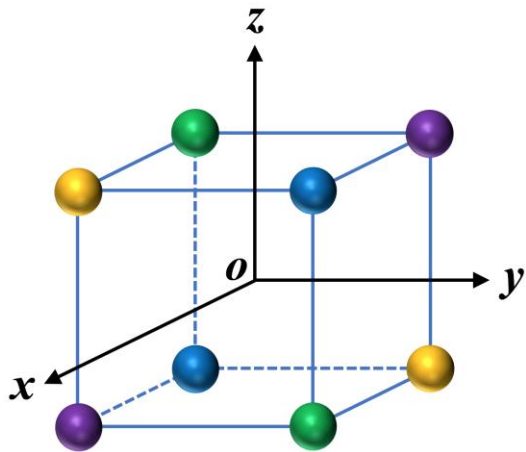
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 2) Inversion (反演)

❖ The inversion operation occurs through a single point (**inversion center**).



$$A_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$x \quad y \quad z \quad \rightarrow \quad -x \quad -y \quad -z$$

(Here, the inversion center is at  $o$ )

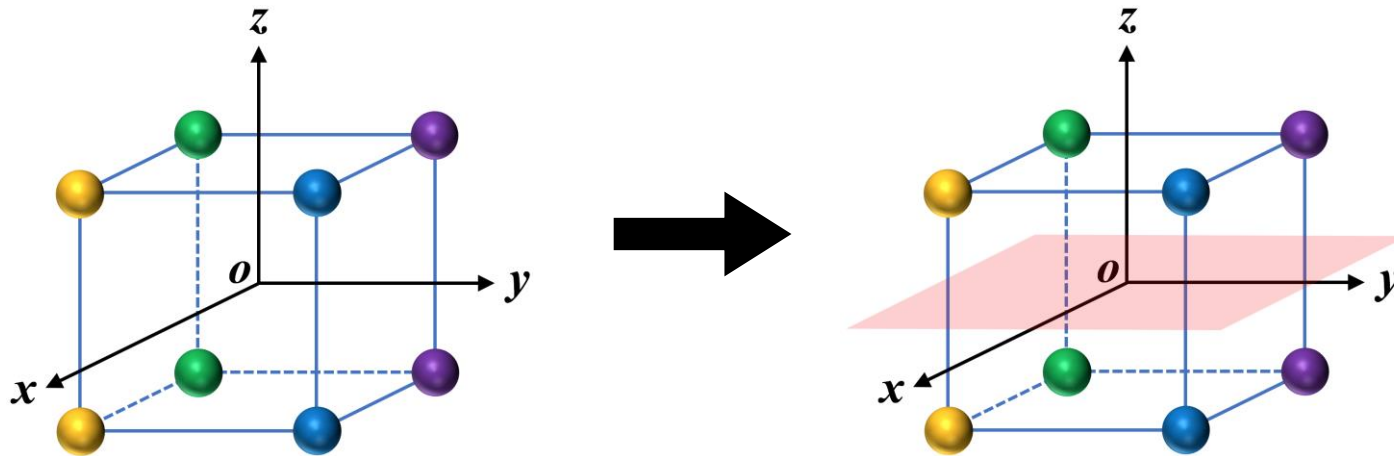
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 3) Reflection (反映)

❖ The reflection operation occurs through a plane (**symmetry plane**) dividing the object.



$$A_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$x \quad y \quad z \quad \rightarrow \quad x \quad y \quad -z$$

(Here, the symmetry plane is the one with  $z = 0$ )

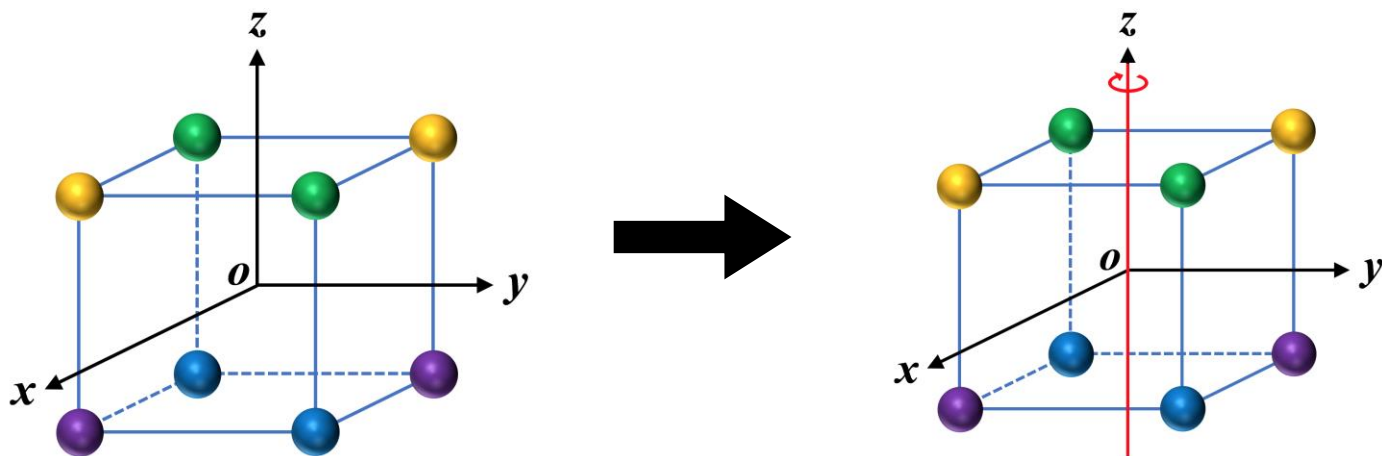
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 4) Proper Rotation (旋转)

- ❖ The proper rotation operation occurs w.r.t. a line (**proper axis**) that the object rotates.
- ❖ The proper axis is ***n*-fold** (***n*次旋转轴**) when rotation by  $2\pi/n$ .



$$A_{ij} = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\begin{matrix} x & y & z \end{matrix} \rightarrow \begin{matrix} x' & y' & z \end{matrix}$$

(Here, the proper axis is the  $z$  axis)

$$x' = x \cos \theta - y \sin \theta$$

$$y' = x \sin \theta + y \cos \theta$$

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 5) Improper Rotation (瑕旋转)

- ❖ The improper rotation operation is a **combination of rotation and reflection/inversion**.
- ❖ It is also called **rotoreflection** (映转) or **rotoinversion** (倒转).



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



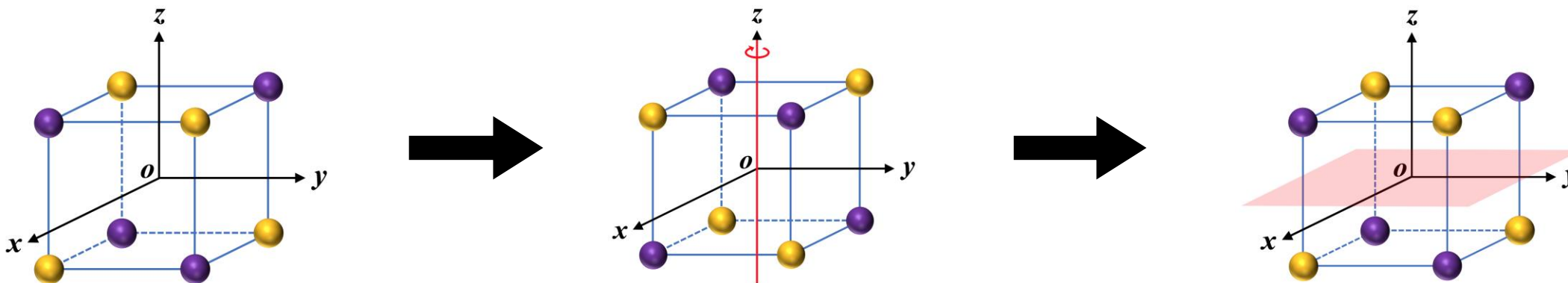
## ➤ Symmetry Operations (对称操作)

### 5) Improper Rotation (瑕旋转)

❖ Rotoreflection (映转):

1) rotation by  $2\pi/n$ ;

2) reflection through a plane perpendicular to the axis.



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



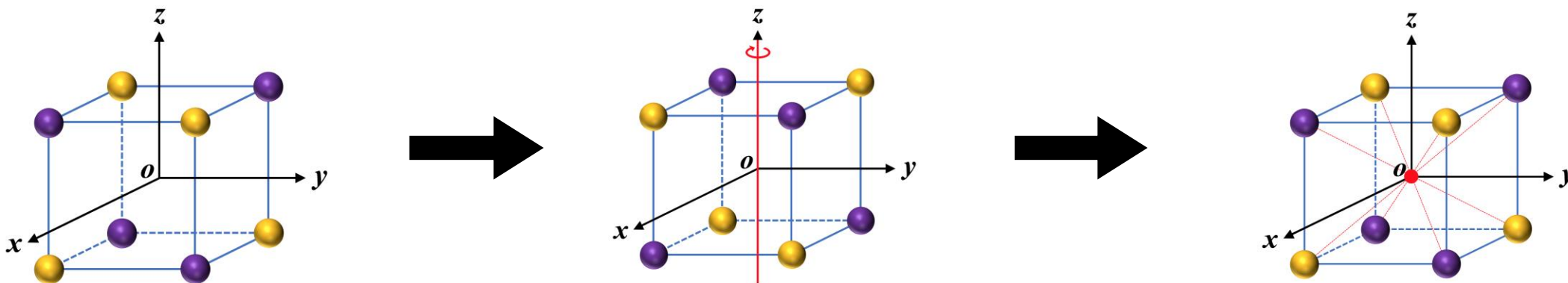
## ➤ Symmetry Operations (对称操作)

### 5) Improper Rotation (瑕旋转)

❖ Rotoinversion (倒转):

1) rotation by  $2\pi/n'$ ;

2) inversion through an inversion center on the axis.



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

### 5) Improper Rotation (瑕旋转)

- ❖ The rotoreflection and rotoinversion are **essentially equivalent!**
- ❖ They are only different in rotation with an angle of  $\pi$ .

Rotoreflexion: 
$$A_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos \theta' & -\sin \theta' & 0 \\ \sin \theta' & \cos \theta' & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} x \ y \ z &\rightarrow x' \ y' \ -z \\ x' &= x \cos \theta' - y \sin \theta' \\ y' &= x \sin \theta' + y \cos \theta' \end{aligned}$$

Rotoinversion: 
$$A_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \cos \theta'' & -\sin \theta'' & 0 \\ \sin \theta'' & \cos \theta'' & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} x \ y \ z &\rightarrow x'' \ y'' \ -z \\ x'' &= x \cos \theta'' - y \sin \theta'' \\ y'' &= x \sin \theta'' + y \cos \theta'' \end{aligned}$$

$$\begin{aligned} x'' &= -x' \\ y'' &= -y' \end{aligned}$$



$$\theta'' = \theta' \pm \pi$$

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Operations (对称操作)

2019级崇新学堂同学“科学可视化”作品



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李宁萍，刘姿含，郭美婧

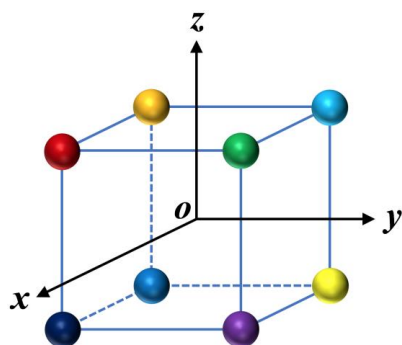
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



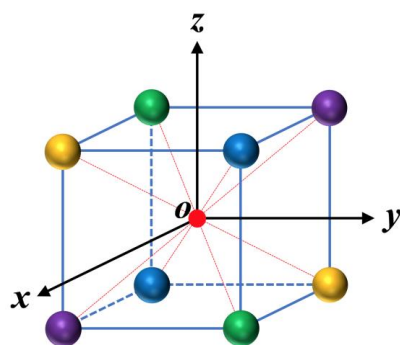
## ➤ Symmetry Elements (对称元素)

- ❖ A symmetry element is a **point of reference** about which symmetry operations can take place.

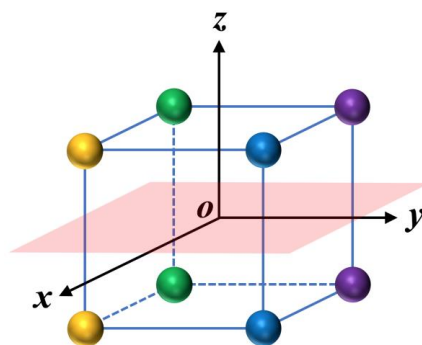
In particular, symmetry elements include:



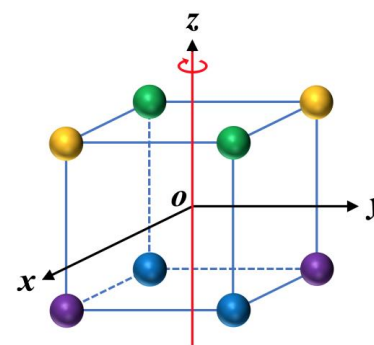
Identity  
(恒等)



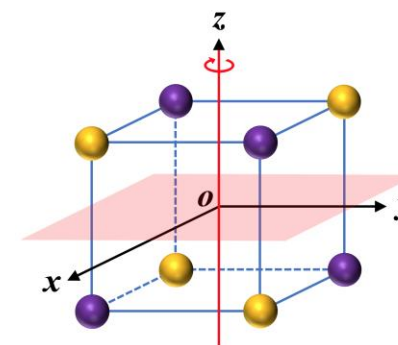
Inversion Center  
(对称中心)



Symmetry Plane  
(对称面)



Proper Axis  
(旋转轴)



Improper Axis  
(反轴)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Elements (对称元素)

Symmetry Operations 对称操作	Symmetry Elements 对称元素	Notation 符号	
		International Notation 国际符号	Schoenflies Notation 熊夫利符号
Identity 恒等	Identity 恒等	<b>1</b>	<b>E</b>
Inversion 反演	Inversion Center 对称中心/反演中心	<b><math>\bar{1}</math></b>	<b>i</b>
Reflection 反映	Symmetry Plane 对称面/反映面	<b>m</b>	<b><math>\sigma</math></b>
Proper Rotation 旋转	Proper Axis 旋转轴	<b>1, 2, 3, 4, 6</b>	<b><math>C_1, C_2, C_3, C_4, C_6</math></b>
Improper Rotation 瑕旋转/映转/倒转	Improper Axis 反轴/映转轴/倒转轴	<b><math>\bar{3}, \bar{4}, \bar{6}</math></b>	<b><math>C_{3i}, S_4, C_{3h}</math></b>

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Elements (对称元素)

❖ In periodic crystals, there are only **8 independent symmetry elements**:

$1, 2, 3, 4, 6, i, m, \bar{4}$

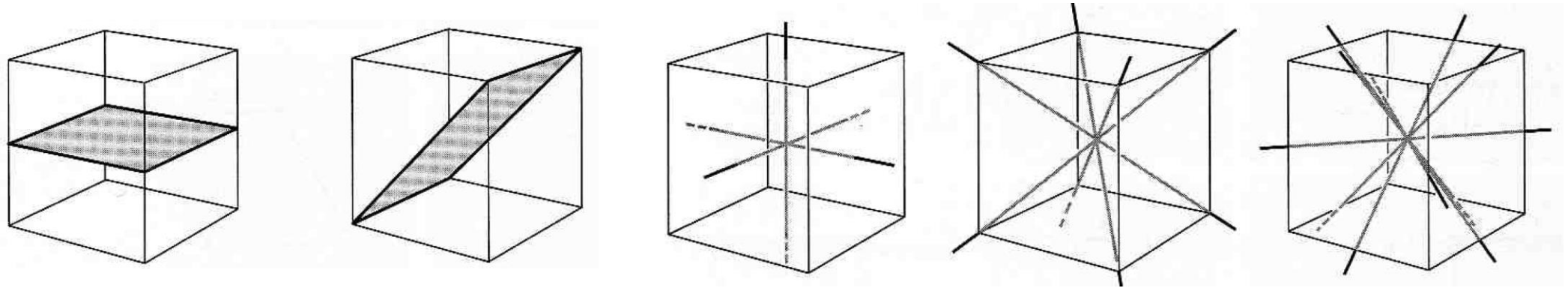
(Note:  $\bar{1} = i$ ,  $\bar{2} = m$ , and  $\bar{3}$  and  $\bar{6}$  are not independent because  $\bar{3} = 3 + i$ ;  $\bar{6} = 3 + m$ )

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Symmetry Elements (对称元素)

- ❖ In practice, for simplicity, only the symmetry elements (instead of the symmetry operations) are listed in order to describe the symmetry properties of a crystal.



The symmetry elements of a cube.

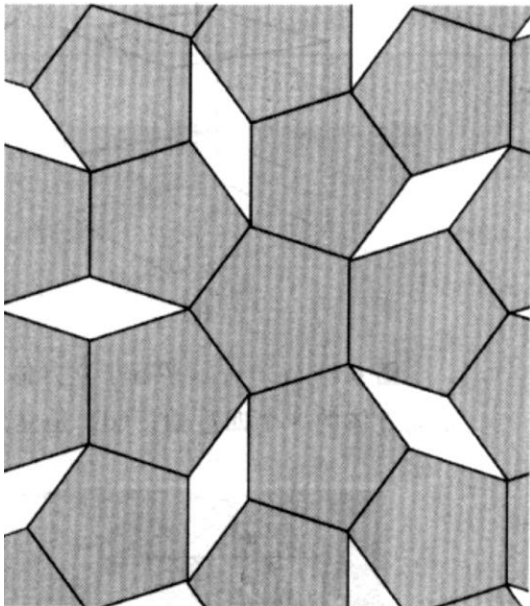


# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Restriction Theorem (晶体学限制定理)

- ❖ The rotational symmetries of a crystal are limited to only 1-fold, 2-fold, 3-fold, 4-fold, and 6-fold, i.e., the **symmetry elements of 1, 2, 3, 4, and 6**. We cannot find a lattice that goes into itself under other rotations, such 5-fold, 7-fold, ...



**Figure 5** A fivefold axis of symmetry cannot exist in a periodic lattice because it is not possible to fill the area of a plane with a connected array of pentagons. We can, however, fill all the area of a plane with just two distinct designs of “tiles” or elementary polygons.

(基泰尔书, page 5)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)

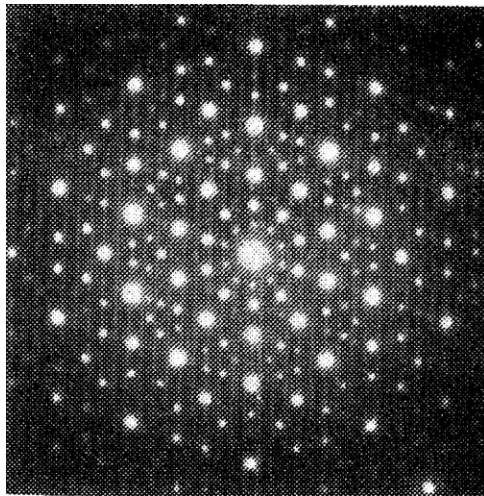


## ➤ Quasicrystal (准晶)

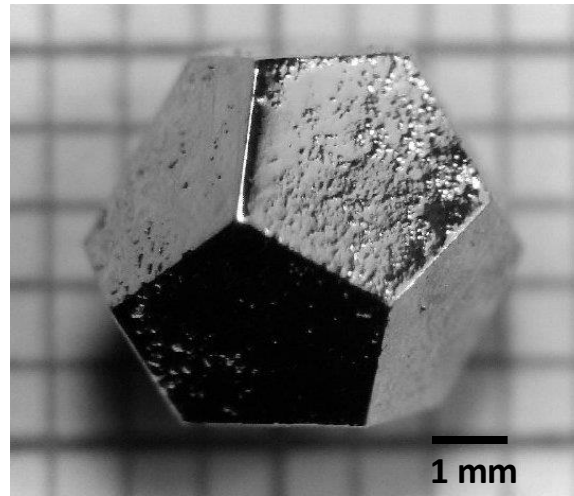
- ❖ The discovery of **quasicrystal (准晶)** in 1984 broke the crystallographic restriction theorem and proved that **there exists 5-fold rotation symmetry in real crystals.**



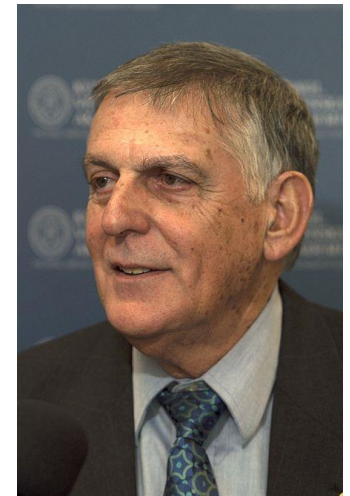
**Nobel Prize in Chemistry 2011**



Electron Diffraction Pattern of  
AlMn Quasicrystal



A Sample of Ho<sub>8.7</sub>Mg<sub>34.6</sub>Zn<sub>56.8</sub>  
Quasicrystal



**Dan Shechtman**  
(1941- )  
Israeli Material Scientist

**D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, *Phys. Rev. Lett.* 53, 1951 (1984).**

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Quasicrystal (准晶)

- ❖ The discovery of **quasicrystal (准晶)** in 1984 broke the crystallographic restriction theorem and proved that **there exists 5-fold rotation symmetry in real crystals**.

	Crystals	
Properties	Periodic Crystals	Quasicrystals
Long-Range Order?	Yes	Yes
Translational Symmetry?	Yes	No
The Crystallographic Restriction Theorem Applies?	Yes	No

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Point Group (晶体学点群)

❖ Mathematically, a **group** (群) is a set (e.g.,  $G$ ) consisting of a group of elements.

$$G = \{ E, A, B, C, D, \dots \}$$

❖ All elements in the group  $G$  satisfy:

1. **Closure** (闭合性): If  $A, B \in G$ , then  $AB = C \in G$

2. **Associativity** (结合律):  $A(BC) = (AB)C$

3. **Identity Element** (单位元素): There exists  $E$  such that all elements meet  $AE = A$

4. **Inverse Element** (逆元素): Each element has an inverse element in the group that  $AA^{-1} = E$

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Point Group (晶体学点群)

- ❖ A crystallographic point group, or **point group** (点群) for short, is a set of symmetry operations that leave at least one point fixed during the operations, i.e., **point symmetry operations** (点对称操作).

$$G = \{1, 2, 3, 4, 6, i, m, \bar{4}\}$$

- ❖ For a periodic crystal, the point group must be consistent with maintenance of the 3D translational symmetry. (注意：“点对称操作”不包含“平移对称操作”).

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Point Group (晶体学点群)

❖ In periodic crystals, the combination of point symmetry operations lead to **32 point groups**.

符号	符号意义	对称类型	数目
$C_n$	具有 $n$ 重旋转对称轴	$C_1, C_2, C_3, C_4, C_6$	5
$C_i$	对称中心 (i)	$C_i (= S_2)$	1
$C_s$	对称面 (m)	$C_s$	1
$C_{nh}$	$h$ 代表除 $n$ 重轴外还有与轴垂直的水平对称面	$C_{2h}, C_{3h}, C_{4h}, C_{6h}$	4
$C_{nv}$	$v$ 代表除 $n$ 重轴外还有通过该轴的铅锤对称面	$C_{2v}, C_{3v}, C_{4v}, C_{6v}$	4
$D_n$	具有 $n$ 重轴和 $n$ 个与之垂直的2重轴	$D_2, D_3, D_4, D_6$	4
$D_{nh}$	$h$ 意义与前同	$D_{2h}, D_{3h}, D_{4h}, D_{6h}$	4
$D_{nd}$	$d$ 表示还有1个平分两个2重轴间夹角的对称面	$D_{2d}, D_{3d}$	2
$S_n$	经 $n$ 重旋转后, 再经垂直该轴的平面镜像	$S_4, S_6$	2
T	4个3重轴和3个2重轴 (四面体对称性)	T	1
$T_h$	$h$ 意义与前同	$T_h$	1
$T_d$	$d$ 意义与前同	$T_d$	1
O	3个互相垂直的4重轴及6个2重轴和4个3重轴	O, $O_h$	2
共计			<b>32</b>

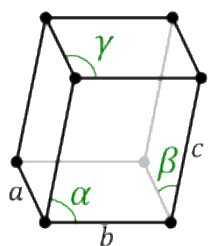


# Chapter 1.2: Symmetry of Crystals (晶体的对称性)

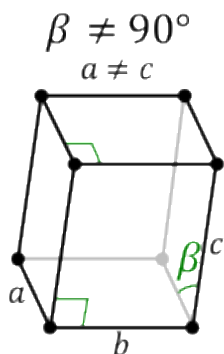


## ➤ Crystal Systems (晶系)

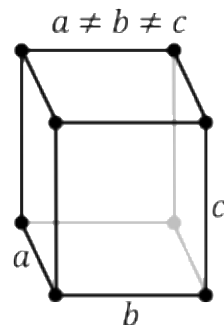
- ❖ Since some symmetry elements may be shared by certain types of crystals, the 32 point groups can be further classified into **7 crystal systems**.



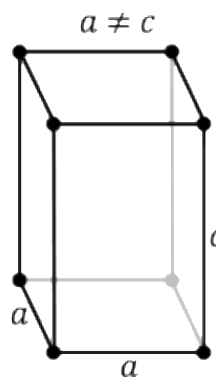
Triclinic  
三斜晶系



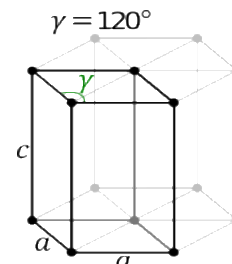
Monoclinic  
单斜晶系



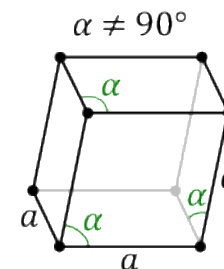
Orthorhombic  
正交晶系



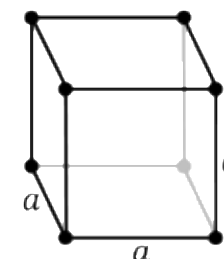
Tetragonal  
四方晶系



Hexagonal  
六方晶系



Rhombohedral  
三方晶系



Cubic  
立方晶系

The unit cells characteristic of the 7 crystal systems.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystal Systems (晶系)

❖ All crystals of each crystal system have the same set of **point groups** and **unit cell**.

Crystal System	晶系	对称性特征	晶胞参数	所属点群
Triclinic	三斜	只有 $C_1$ 或 $C_i$	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	$C_1$ 、 $C_i$
Monoclinic	单斜	唯一 $C_2$ 或 $C_s$	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$	$C_2$ 、 $C_s$ 、 $C_{2h}$
Orthorhombic	正交	三个 $C_2$ 或 $C_s$	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$D_2$ 、 $C_{2v}$ 、 $D_{2h}$
Rhombohedral	三方	唯一 $C_3$ 或 $S_6$	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	$C_3$ 、 $S_6$ 、 $D_3$ $C_{3v}$ 、 $D_{3d}$
Tetragonal	四方	唯一 $C_4$ 或 $S_4$	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$C_4$ 、 $S_4$ 、 $C_{4h}$ 、 $D_4$ $C_{4v}$ 、 $D_{2d}$ 、 $D_{4h}$
Hexagonal	六方	唯一 $C_6$ 或 $S_3$	$a = b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$	$C_6$ 、 $C_{3h}$ 、 $C_{6h}$ 、 $D_6$ 、 $C_{6v}$ 、 $D_{3h}$ 、 $D_{6h}$
Cubic	立方	四个 $C_3$	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	$T$ 、 $T_h$ 、 $T_d$ $O$ 、 $O_h$



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Bravais Lattices (布拉维格子)

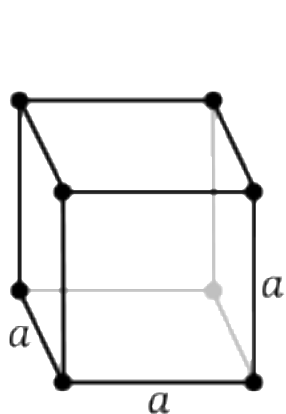
- ❖ By considering how the lattice sites are located in the unit cells of the 7 crystal systems, it ends up with **14 Bravais lattices** in 3D.
- ❖ **Any real periodic crystal corresponds to one of the 14 Bravais lattices!**

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)

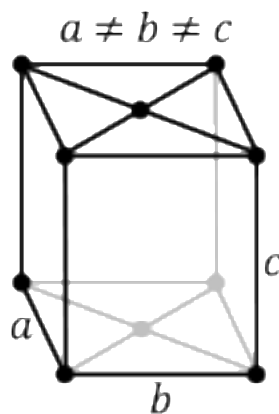


## ➤ Bravais Lattices (布拉维格子)

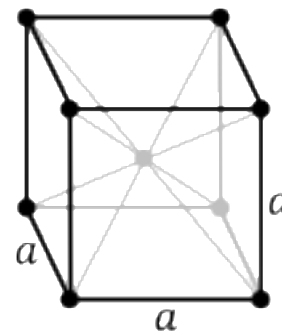
❖ There are 4 centering types identifying the location of the lattice sites in the unit cell:



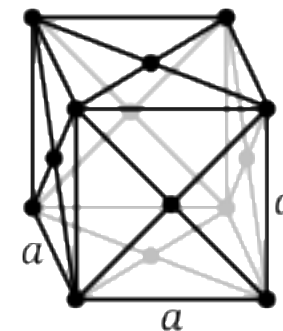
Primitive (P)  
原始格子



Base-centered (C)  
底心格子



Body-centered (I)  
体心格子



Face-centered (F)  
面心格子

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Bravais Lattices (布拉维格子)

❖ The 14 Bravais lattices in 3D:

晶系	原始格子(P)	底心格子(C)	体心格子(I)	面心格子(F)	合计
三斜		$C = I$	$I = F$	$F = P$	1
单斜			$I = F$	$F = C$	2
正交					4
四方		$C = P$		$F = I$	2
三方		与本晶系 对称不符	$I = F$	$F = P$	1
六方		与本晶系 对称不符	与空间格子的 条件不符	与空间格子的 条件不符	1
立方		与本晶系 对称不符			3

共计14

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)

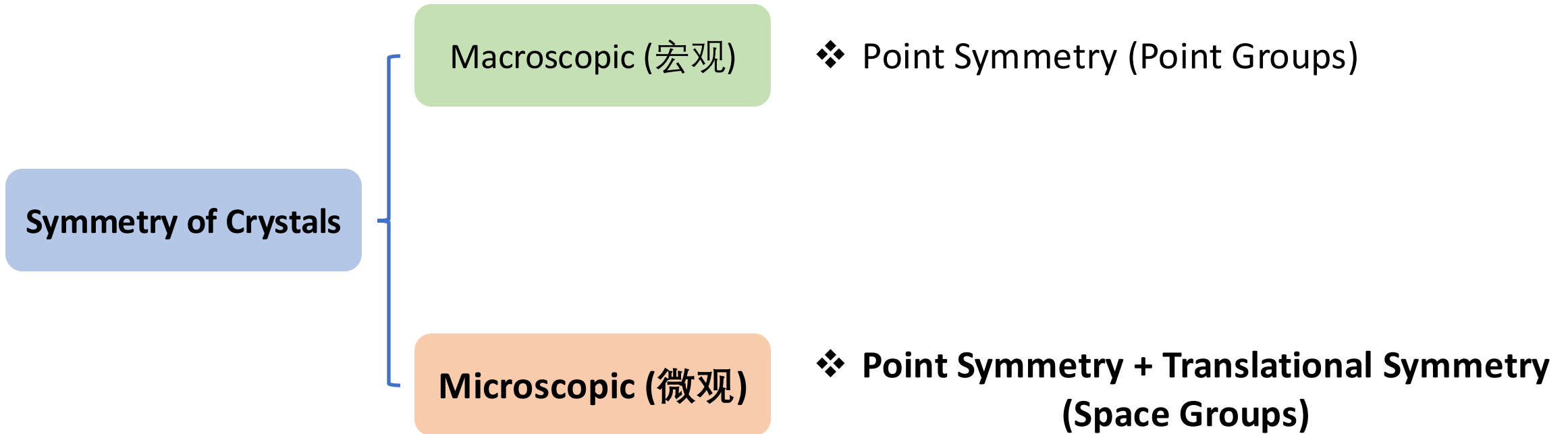


## Microscopic Symmetry of Crystals (晶体的微观对称性)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Microscopic Symmetry of Crystals (晶体的微观对称性)

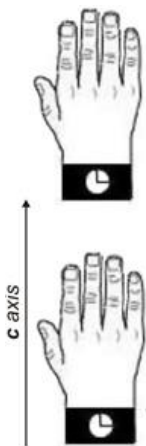


# Chapter 1.2: Symmetry of Crystals (晶体的对称性)

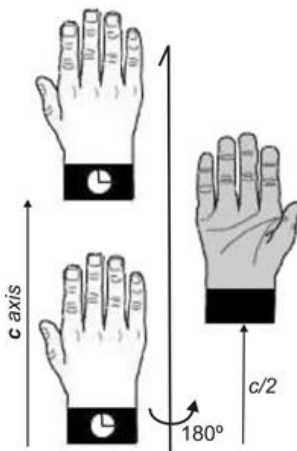


## ➤ Translational Symmetry (平移对称性)

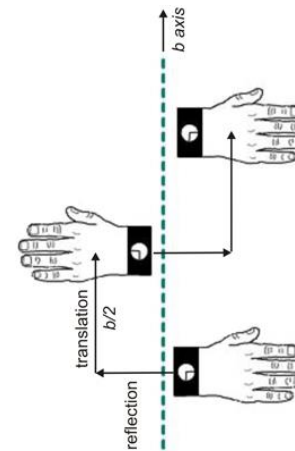
- ❖ The translational symmetry can be described in terms of **translational symmetry elements** and the corresponding **translational symmetry operations**.
- ❖ The translational symmetry elements include:



Translation Axis (平移轴)



Screw Axis (螺旋轴)



Glide Plane (滑移面)

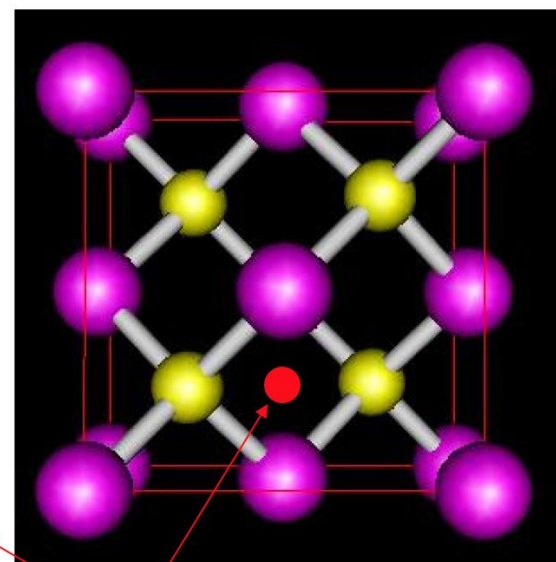
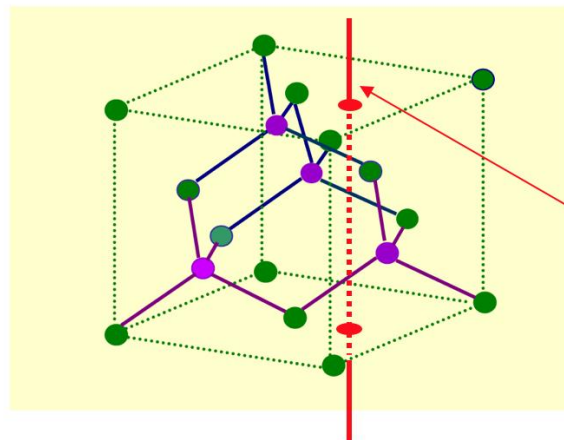
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Translational Symmetry (平移对称性)

### 金刚石结构中的4度螺旋轴

取上下底面心的连线,再沿单胞边长平移 $a/4$ 就是一个4度螺旋轴。晶体绕该轴转 $90^\circ$ 后,再沿该轴平移 $a/4$ ,能自身重合。



4度螺旋轴

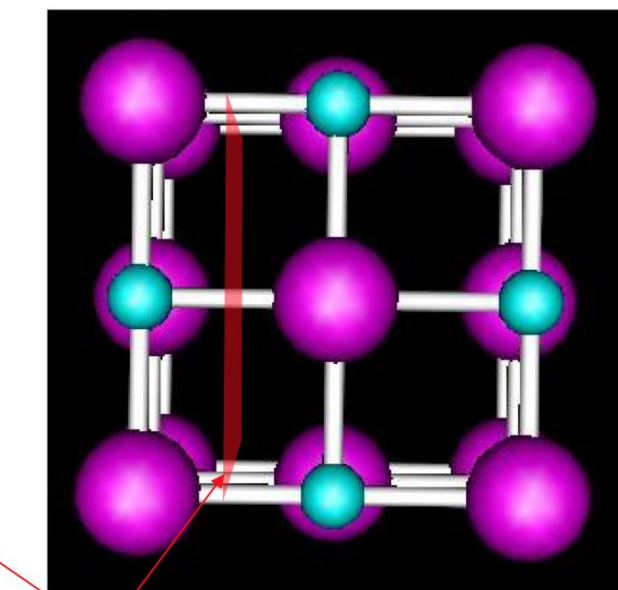
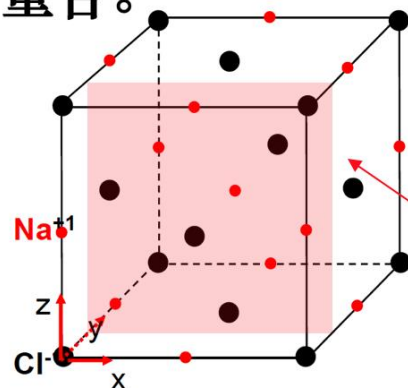
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Translational Symmetry (平移对称性)

### 氯化钠结构中的滑移反映面

取氯和钠的中垂面为镜面，再沿平行于该面的原子排列方向平移 $a/2$ ，能自身重合。



滑移反映面



# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Space Group (晶体学空间群)

- ❖ The translational symmetry operations give rise to **14 translation groups** (平移群, as many as the number of Bravais lattices).
- ❖ In 3D periodic crystals, the combination of **point symmetry operations** and **translational symmetry operations** lead to **230 crystallographic space groups**.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Crystallographic Space Group (晶体学空间群)

表 2.3 7 个晶系, 14 个布拉维格子和 73 个简单空间群

晶系	单胞基矢特性	布拉维格子	空间群
三斜	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	简单三斜(P)	$P1, P\bar{1}$
单斜	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	简单单斜(P)	$P2, Pm, P2/m$
		底心单斜(B或A)	$B2, Bm, B2/m$
正交	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	简单正交(P)	$P222, Pmm2, Pmmm$
		底心正交(C, A或B)	$C222, Cmm2, Amm2, Cmmm$
		体心正交(I)	$I222, Immm, Immm$
		面心正交(F)	$F222, Fmm2, Fmmm$
四方	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	简单四方(P)	$P4, P\bar{4}, P4/m, P422, P4mm, P42m, P\bar{4}m2, P4/mmm$
		体心四方(I)	$I4, I\bar{4}, I4/m, I422, I4mm, I\bar{4}2m, I\bar{4}m2, I4/mmm$
三角	$a = b = c$ $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$	三角(R,P)	$R3, R\bar{3}, R32, R3m, R\bar{3}m, P3, P\bar{3}, P312, P321, P3m1, P31m, P\bar{3}1m, P\bar{3}m1$
六角	$a = b \neq c$ $\alpha = \beta = 90^\circ; \gamma = 120^\circ$	六角(P)	$P6, P\bar{6}, P6/m, P622, P6mm, P\bar{6}m2, P\bar{6}2m, P6/mmm$
立方	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	简单立方(P)	$P23, Pm3, P432, P\bar{4}3m, Pm3m$
		体心立方(I)	$I23, Im3, I432, I\bar{4}3m, Im3m$
		面心立方(F)	$F23, Fm3, F432, F\bar{4}3m, Fm3m$

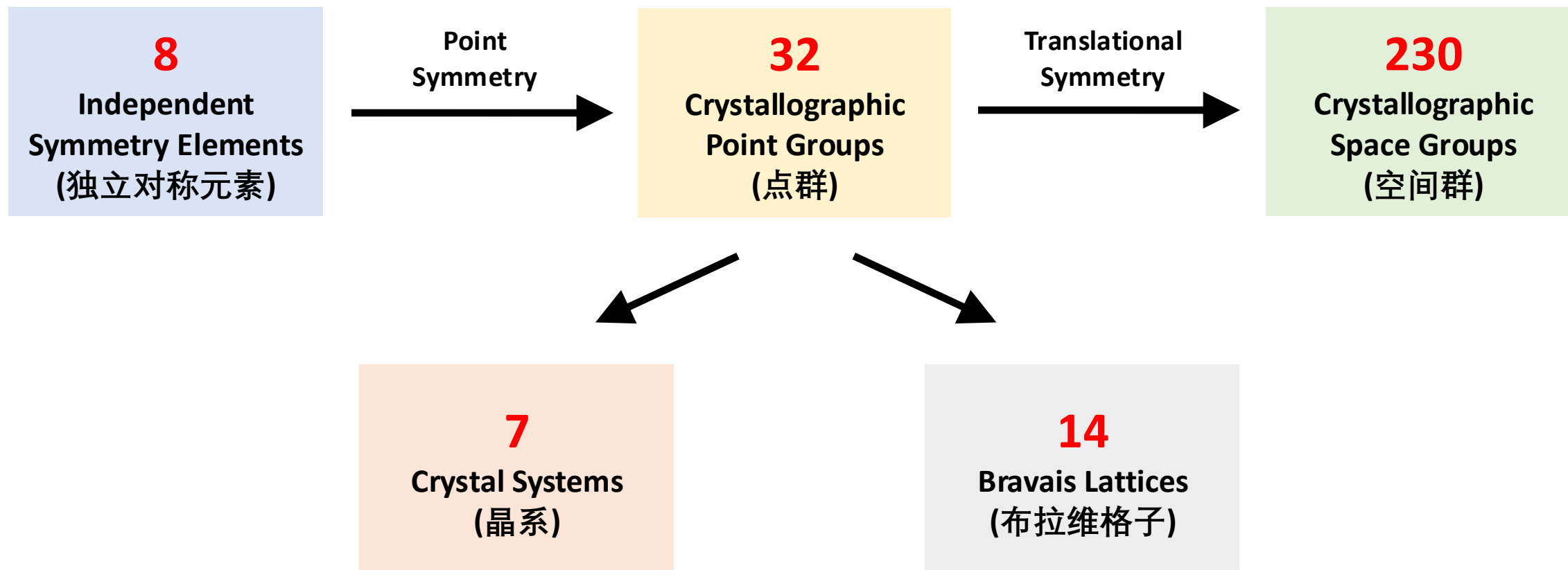
- ❖ Space groups can be used to give **more detailed classifications** of real crystals.
- ❖ Not all space groups have found examples of real crystals.

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ The Case of 3D

❖ In **3D periodic crystals**, there exist:

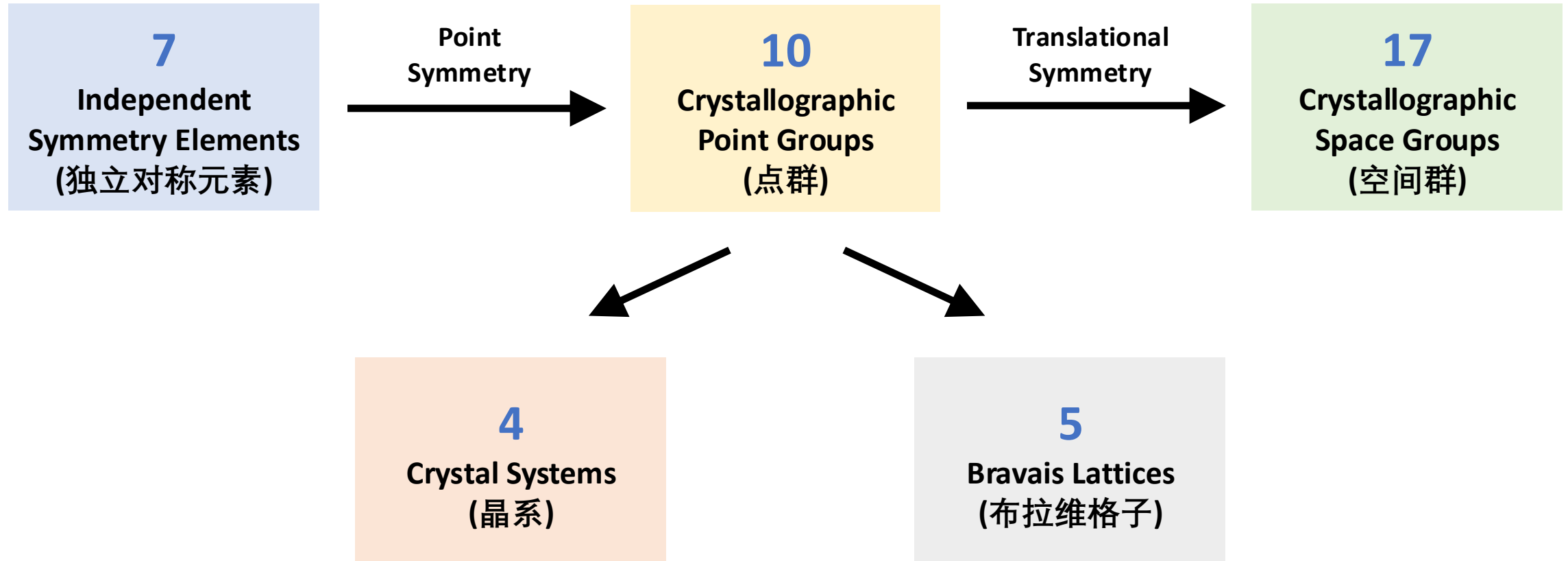


# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ The Case of 2D

❖ In 2D periodic crystals, there exist:



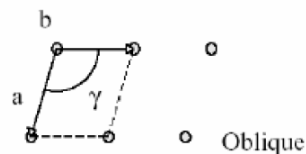
# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ The Case of 2D

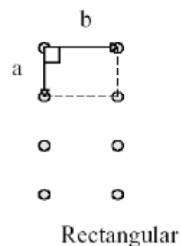
### ❖ 4 Crystal Systems and 5 Bravais Lattices:

斜方

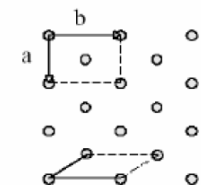


$$a \neq b, \gamma \neq 90^\circ$$

长方



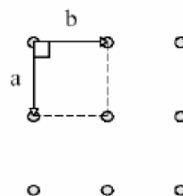
Rectangular



Centered Rectangular

$$a \neq b, \gamma = 90^\circ$$

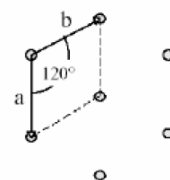
正方



Square

$$a = b, \gamma = 90^\circ$$

六角



Hexagonal

$$a = b, \gamma = 120^\circ$$



### Summary (总结)

# Chapter 1.2: Symmetry of Crystals (晶体的对称性)



## ➤ Summary (总结)

### ❖ Symmetry of Crystals:

- 1) Macroscopic symmetry;
- 2) Microscopic symmetry

### ❖ Macroscopic Symmetry:

- 1) Symmetry Operations;
- 2) Symmetry Elements;
- 3) Point Group;
- 4) Crystal Systems;
- 5) Bravais Lattices.

### ❖ Microscopic Symmetry.



1. 列出硅(silicon)晶体所属的点群、晶系、布拉维格子等信息，并在单胞中画出可能的点对称元素。
2. 用 Materials Studio 软件画出硅晶体的一个单胞（截图到作业纸上），标出任意一条4度螺旋轴，并熟悉 Materials Studio 软件的使用。

(Materials Studio 下载链接: <https://pan.baidu.com/s/1zQ5qVycOEhFmpxZZTpTZWQ?pwd=m8m5> 提取码: m8m5)

提交时间：3月3日之前

提交方式：手写（写明姓名学号）后拍照，通过本班课代表统一提交电子版