



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)

- To understand the concepts of **reciprocal lattice**;
- To understand the connection between a reciprocal lattice and its direct lattice;
- To learn the typical reciprocal lattices.



Reciprocal Lattice (倒格子)

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice (倒格子)

❖ Assuming that we define **two sets of lattices**:

Lattice 1:

Basis Vectors (基矢):

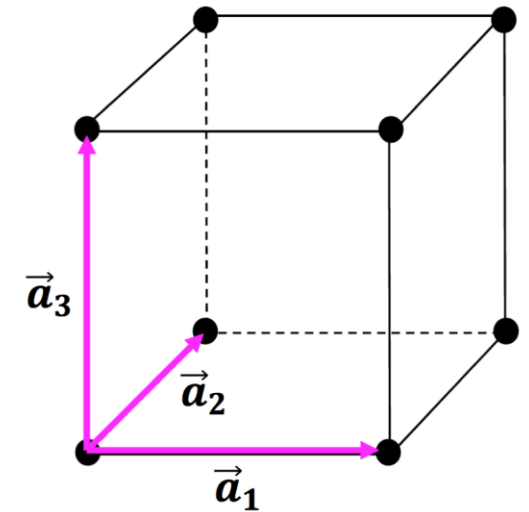
$$\vec{a}_1, \vec{a}_2, \text{ and } \vec{a}_3$$

Lattice Vectors (格矢):

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

Cell Volume (晶胞体积):

$$\Omega = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$



Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice (倒格子)

❖ Assuming that we define **two sets of lattices**:

Lattice 2:

Basis Vectors (基矢):

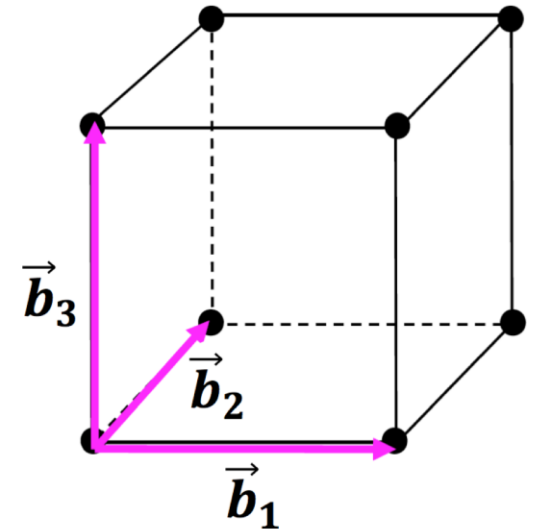
$$\vec{b}_1, \vec{b}_2, \text{ and } \vec{b}_3$$

Lattice Vectors (格矢):

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

Cell Volume (晶胞体积):

$$\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$



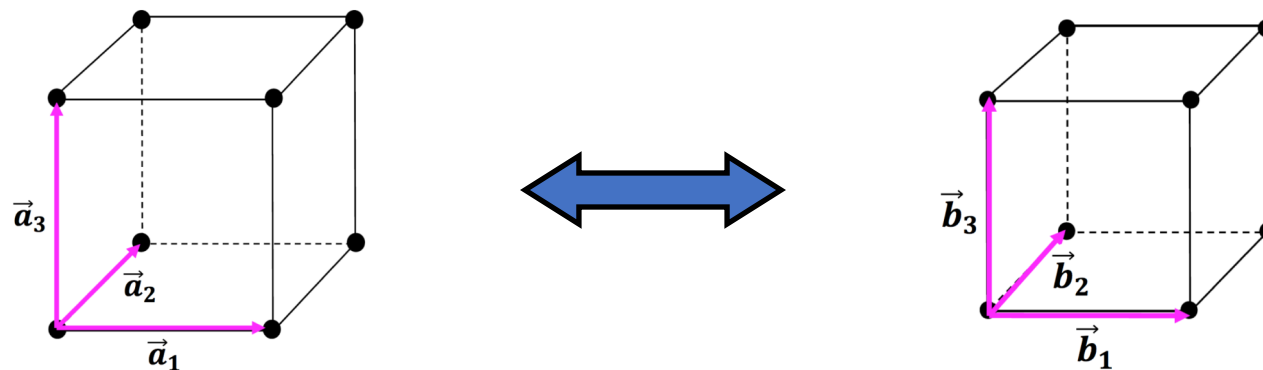
Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice (倒格子)

- ❖ The two sets of lattices defined above are **reciprocal to each other** (互为正倒格子) if the following is satisfied:

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} = \begin{cases} 2\pi, & i = j \\ 0, & i \neq j \end{cases} \quad i, j = 1, 2, 3$$



Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice (倒格子)

❖ If the lattice defined by \vec{R} is called **direct lattice** (正格子), the one defined by \vec{G} is called **reciprocal lattice** (倒格子, 或“倒易点阵”), or *vice versa*.

❖ The space in which the **direct lattice** is defined is called **real space** (实空间).

The space in which the **reciprocal lattice** is defined is called **reciprocal space** (倒空间).

❖ The lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ defining the reciprocal lattice is called **reciprocal lattice vector** (倒格矢).

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice (倒格子)

❖ Alternatively, the **basis vectors of reciprocal lattice** can be defined as:

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

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

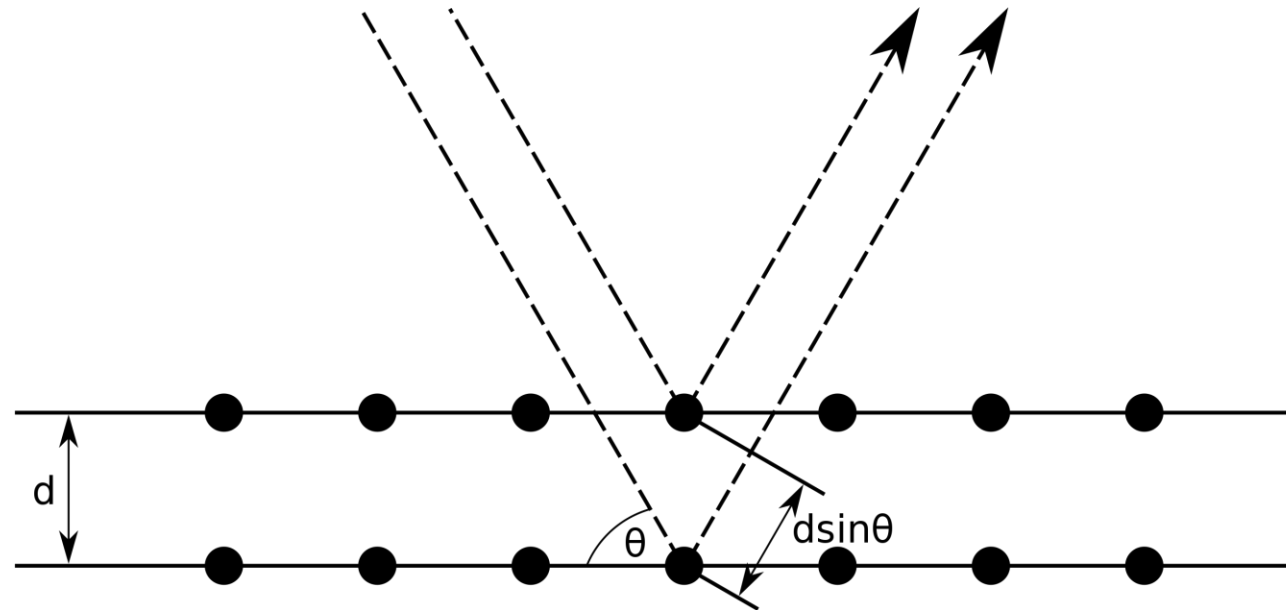
$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\Omega}$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice and the Bragg Law (倒格子与布拉格定律)

❖ The **Bragg law** is the condition for **Bragg diffraction** (布拉格衍射):



Bragg Diffraction

Chapter 1.4: Reciprocal Lattice (倒易点阵)

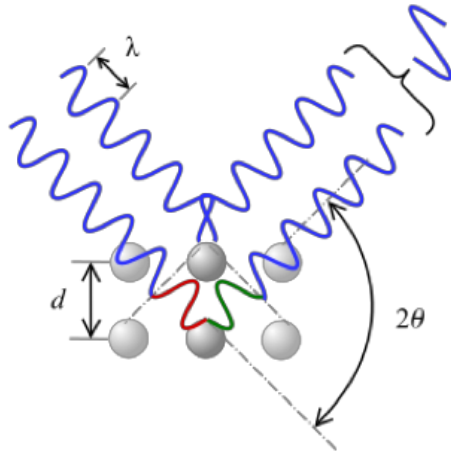


➤ Reciprocal Lattice and the Bragg Law (倒格子与布拉格定律)

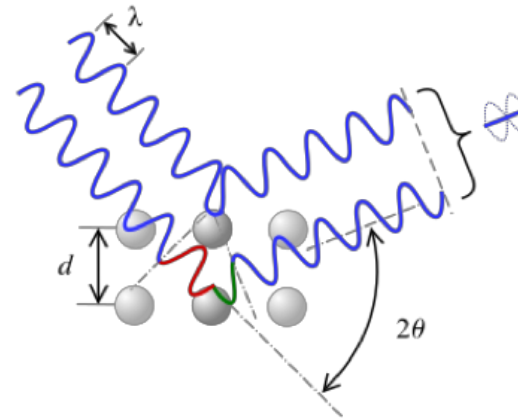
❖ The **Bragg law** is the condition for **Bragg diffraction** (布拉格衍射):

$$2d \sin \theta = n\lambda$$

(n is an integer and $\lambda \leq 2d$)



Constructive Interference
(相长干涉)



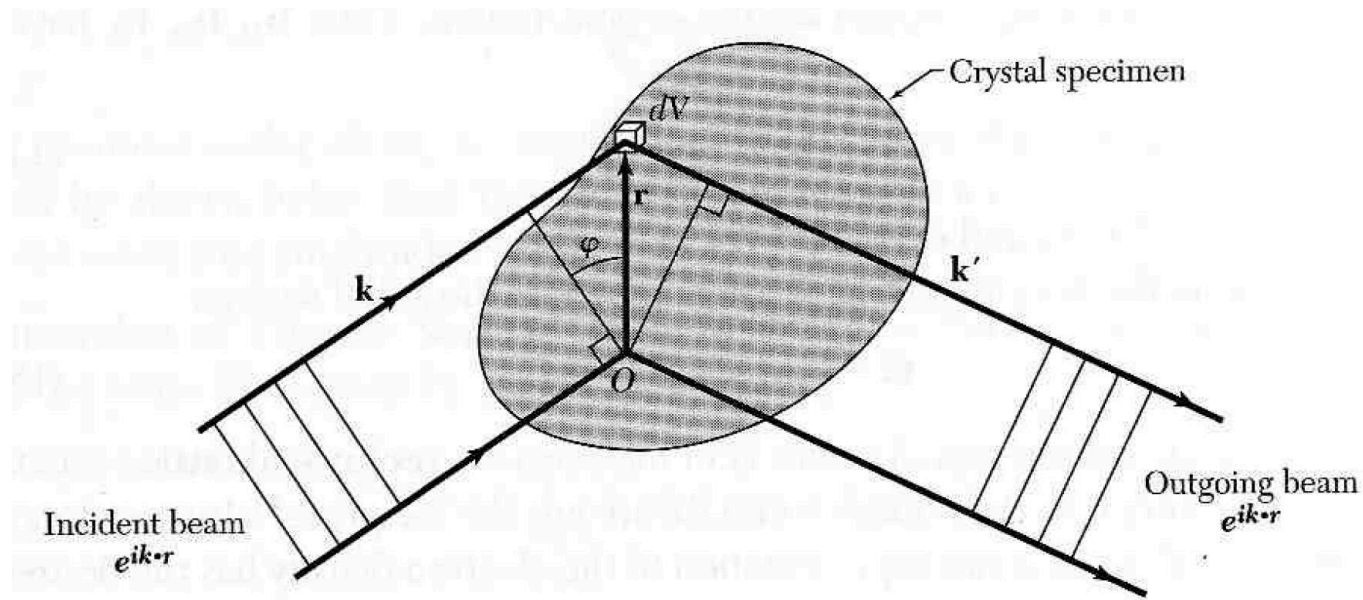
Destructive Interference
(相消干涉)

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice and the Bragg Law (倒格子与布拉格定律)

❖ Laue condition for the diffraction (劳厄衍射条件):



\vec{k} : wave vector of the incident beam.

\vec{k}' : wave vector of the outgoing beam.

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Reciprocal Lattice and the Bragg Law (倒格子与布拉格定律)

❖ Laue condition for the diffraction (劳厄衍射条件):

The possible reflection is determined by a set of reciprocal lattice vectors \vec{G} that satisfy:

$$\vec{k}' - \vec{k} = \vec{G} \quad \xrightarrow{k' = k} \quad \boxed{2\vec{k} \cdot \vec{G} = G^2}$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

1) The basis vectors are orthogonal:

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$\delta_{ij} = \begin{cases} 2\pi, & i = j \\ 0, & i \neq j \end{cases} \quad i, j = 1, 2, 3$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

2) The dot product of the lattice vectors is an integral multiple of 2π :

$$\vec{R} \cdot \vec{G} = 2\pi m \quad (m \text{ is an integer})$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

3) The volumes of the primitive cells satisfy:

$$\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\Omega}$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

- 4) The reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is perpendicular to the crystal planes (hkl) of the direct lattice, and the interplanar spacing (晶面间距) d_{hkl} can be written as:

$$d_{hkl} = \frac{2\pi}{|\vec{G}|}$$

Conclusion: A lattice vector in the reciprocal lattice corresponds to a family of crystal planes in the direct lattice:

- 1) The direction of the vector is parallel to the normal direction of the planes;
- 2) The magnitude of the vector is 2π times of the reciprocal of interplanar spacing.

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

- 5) The direct lattice and the reciprocal lattice are reciprocal to each other, i.e., the reciprocal lattice of a reciprocal lattice is its direct lattice.

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

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

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



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

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

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

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

6) The direct lattice and reciprocal lattice of the same crystal have the same point group symmetry.

Proof

Assuming α is a symmetry operation of a point group, for a direction lattice vector \vec{R} , it is obvious that $\alpha\vec{R}$ and $\alpha^{-1}\vec{R}$ are both direct lattice vectors. Thus:

$$\vec{G} \cdot \vec{R} = 2\pi m \quad \longrightarrow \quad \vec{G} \cdot \alpha\vec{R} = 2\pi m \quad \vec{G} \cdot \alpha^{-1}\vec{R} = 2\pi m$$

Since α is orthogonal transformation, we obtain:

$$\alpha\vec{G} \cdot \vec{R} = \alpha\vec{G} \cdot \alpha\alpha^{-1}\vec{R} = \vec{G} \cdot \alpha^{-1}\vec{R} = 2\pi m$$

$$\alpha^{-1}\vec{G} \cdot \vec{R} = \alpha^{-1}\vec{G} \cdot \alpha^{-1}\alpha\vec{R} = \vec{G} \cdot \alpha\vec{R} = 2\pi m$$

Therefore, for any symmetry operation α of a point group, $\alpha\vec{G}$ and $\alpha^{-1}\vec{G}$ are also reciprocal lattice vectors.

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ The Physical Meaning of Reciprocal Lattice (倒格子的物理意义)

- ❖ The reciprocal lattice is the **Fourier Transform** of the direct lattice.
- ❖ The direct lattice is the **inverse Fourier Transform** of the reciprocal lattice.

$$F(\vec{r}) = \sum_{\vec{G}_{hkl}} A(\vec{G}_{hkl}) e^{i\vec{G}_{hkl} \cdot \vec{r}}$$

$$A(\vec{G}_{hkl}) = \frac{1}{\Omega} \int F(\vec{r}) e^{-i\vec{G}_{hkl} \cdot \vec{r}} d\vec{r}$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ The Physical Meaning of Reciprocal Lattice (倒格子的物理意义)

- ❖ Each crystal structure corresponds to **2 sets of lattices**, i.e., the **direct lattice** (Bravais lattice) and the **reciprocal lattice**.
 - The **direct lattice** shows the periodic array of atoms in real space;
 - The **reciprocal lattice** shows the periodicity of physical properties in reciprocal space.



Examples of Reciprocal Lattice (倒格子实例)

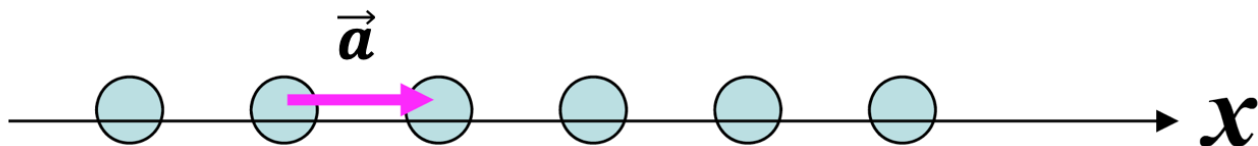
Chapter 1.4: Reciprocal Lattice (倒易点阵)



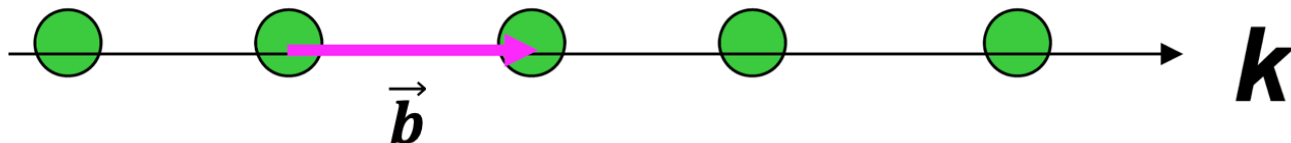
➤ Examples of Reciprocal Lattice

❖ 1D

Direct Lattice



Reciprocal Lattice



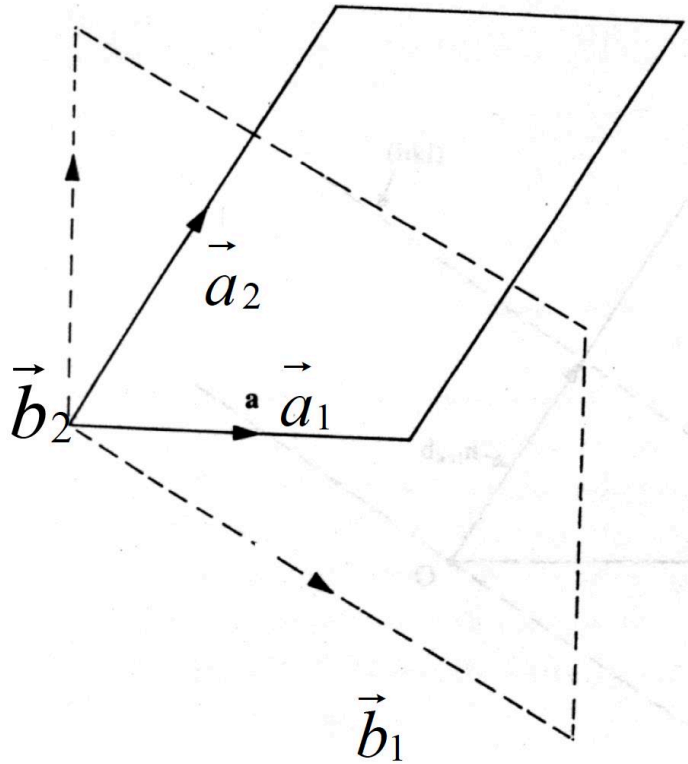
$$b = 2\pi/a \qquad \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

❖ 2D



$$\vec{b}_1 \perp \vec{a}_2$$

$$\vec{b}_2 \perp \vec{a}_1$$

$$\vec{b}_1 \cdot \vec{a}_1 = \vec{b}_2 \cdot \vec{a}_2 = 2\pi$$

$$\vec{b}_1 \cdot \vec{a}_2 = \vec{b}_2 \cdot \vec{a}_1 = 0$$

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

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

Here, " \vec{a}_3 " is the normal vector perpendicular to the 2D plane.

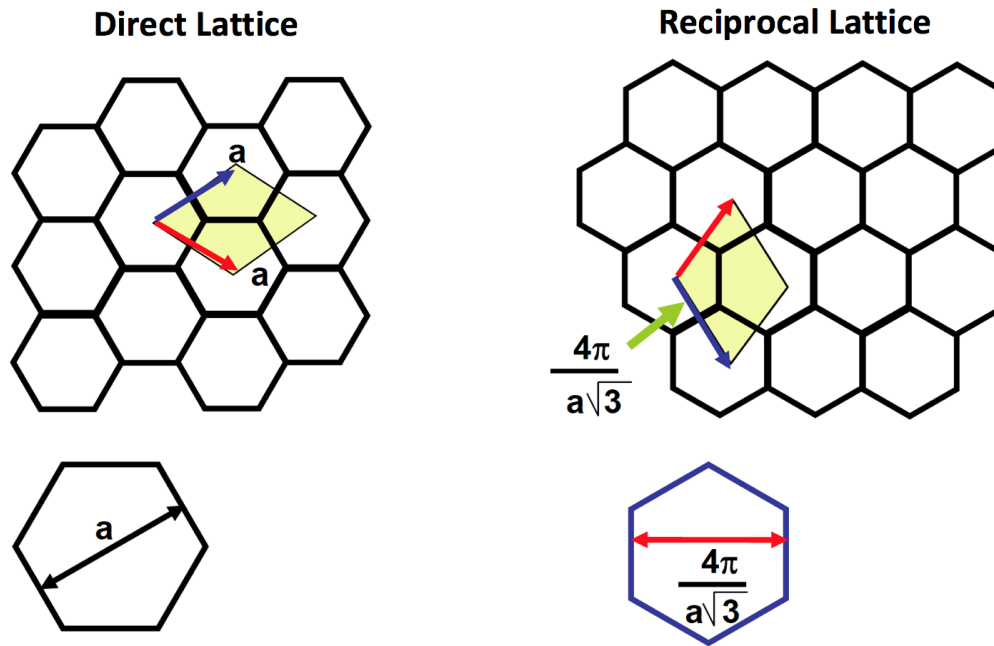
Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

❖ 2D

Example: **Graphene**



Here, " \vec{a}_3 " is the normal vector perpendicular to the 2D plane.

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

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

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

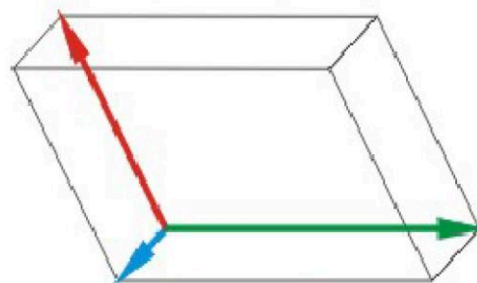
❖ 3D- Simple Lattice (简单晶格)

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

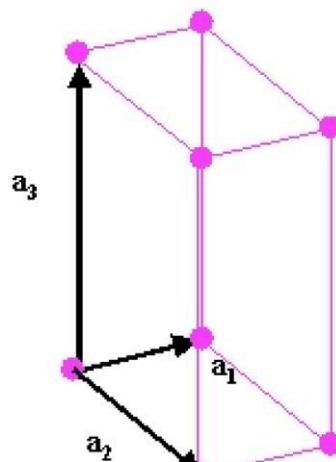
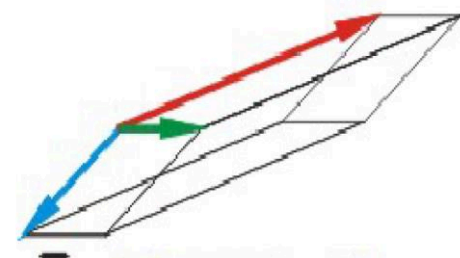
$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

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

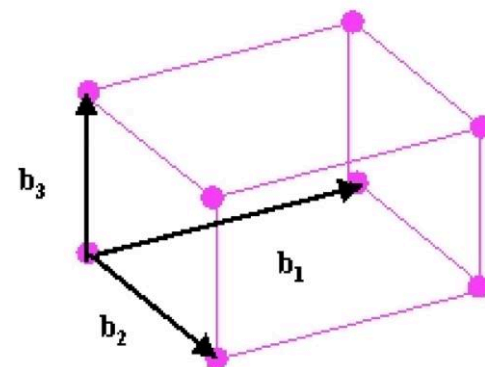
Direct Lattice



Reciprocal Lattice



Simple Orthorhombic Bravais Lattice
with $a_3 > a_2 > a_1$



Reciprocal Lattice
Note: $b_1 > b_2 > b_3$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



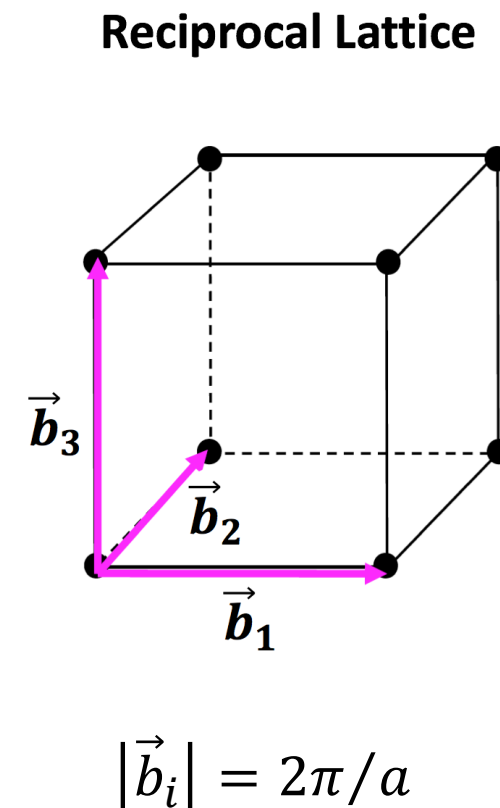
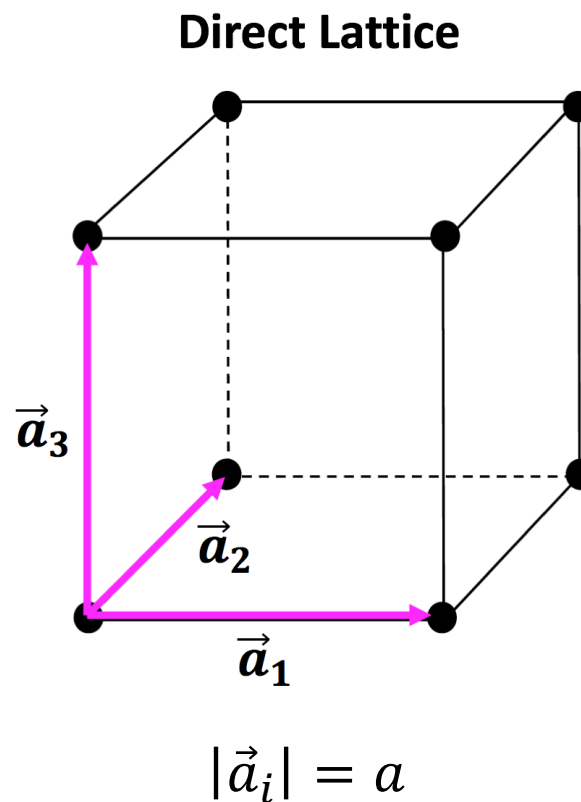
➤ Examples of Reciprocal Lattice

❖ 3D- *sc* Lattice (简单立方晶格)

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

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

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



Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

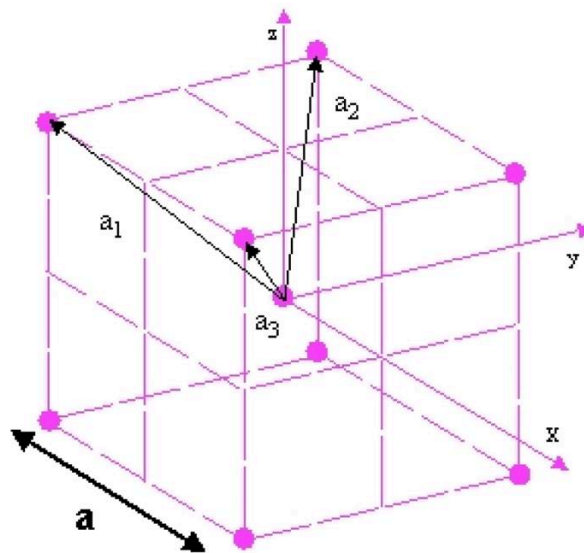
❖ 3D- *bcc* Lattice (体心立方晶格)

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

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

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

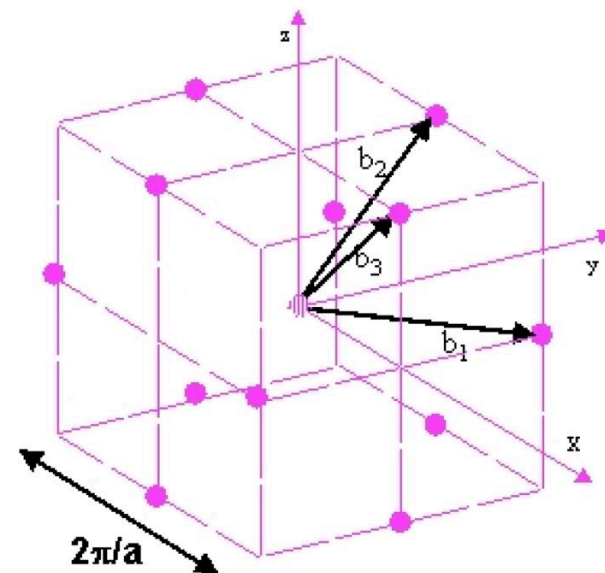
Direct Lattice



Primitive vectors and the conventional cell of bcc lattice

bcc

Reciprocal Lattice



Reciprocal lattice is Face Centered Cubic

fcc

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

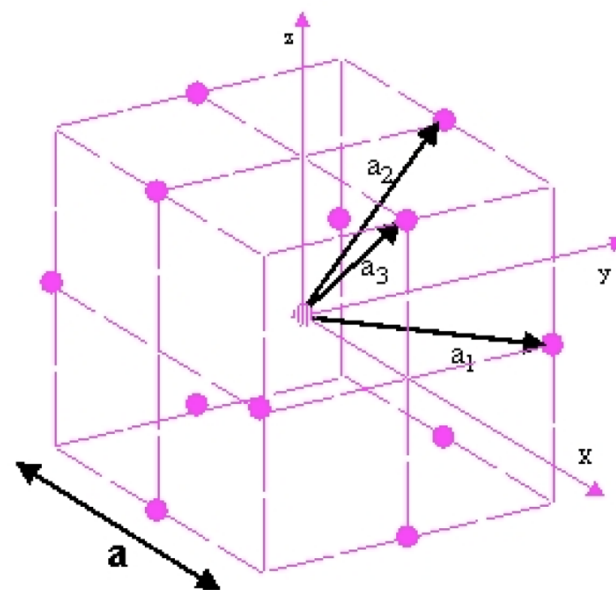
❖ 3D-*fcc* Lattice (面心立方晶格)

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

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

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

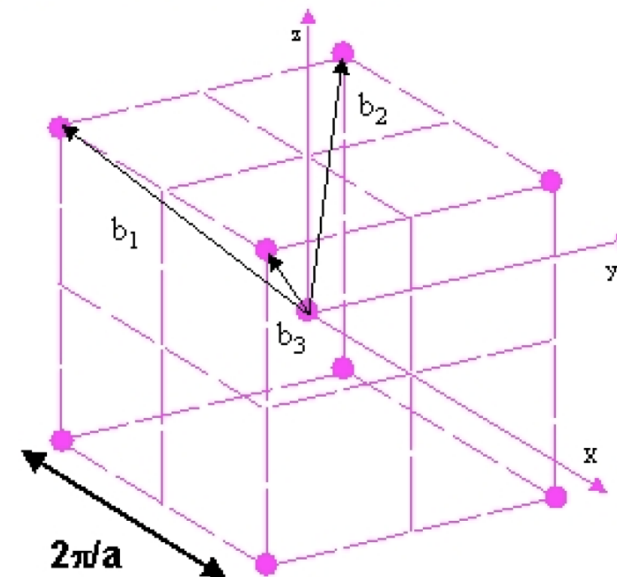
Direct Lattice



Primitive vectors and the
conventional cell of fcc lattice

fcc

Reciprocal Lattice



Reciprocal lattice is
Body Centered Cubic

bcc

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

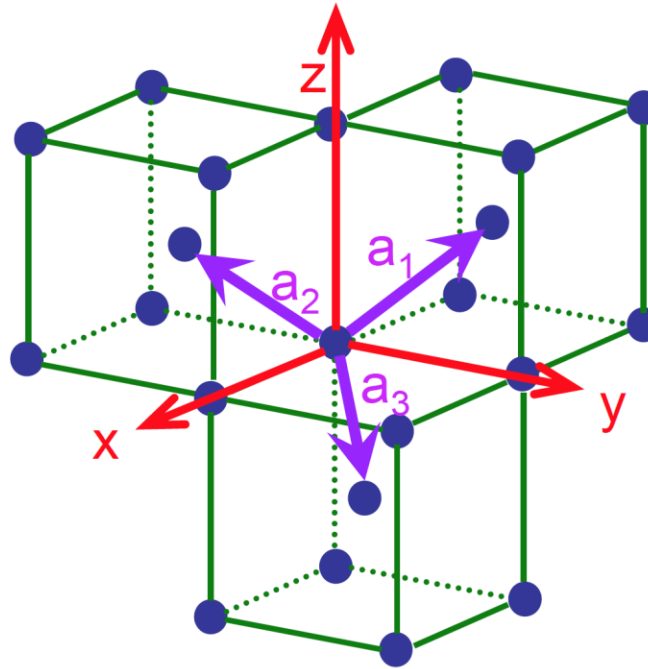
bcc lattice

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

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

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

$$\Omega = a^3/2$$



fcc lattice

$$\vec{b}_1 = \frac{2\pi}{a}(\vec{y} + \vec{z})$$

$$\vec{b}_2 = \frac{2\pi}{a}(\vec{z} + \vec{x})$$

$$\vec{b}_3 = \frac{2\pi}{a}(\vec{x} + \vec{y})$$

$$\Omega^* = 16(\pi/a)^3$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Examples of Reciprocal Lattice

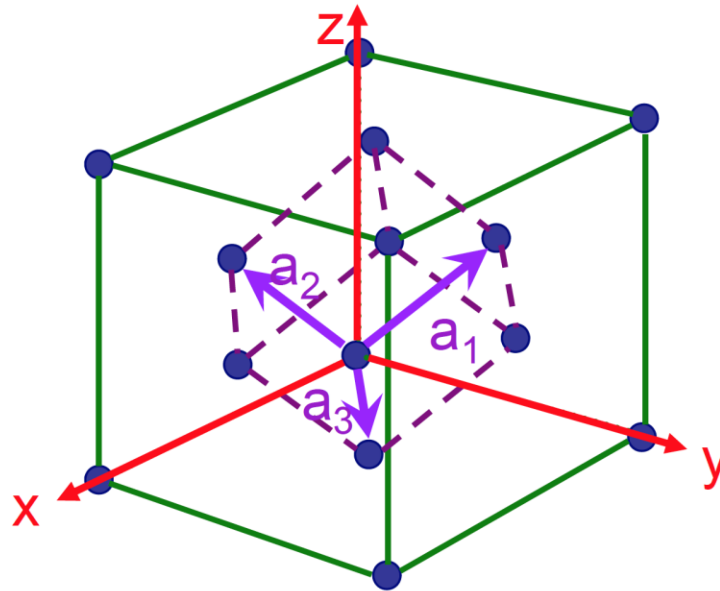
fcc lattice

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

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

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

$$\Omega = a^3/4$$



bcc lattice

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

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

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

$$\Omega^* = 32(\pi/a)^3$$



Brillouin Zones (布里渊区)

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ In general, **Brillouin zones** are defined in the reciprocal space as follows:

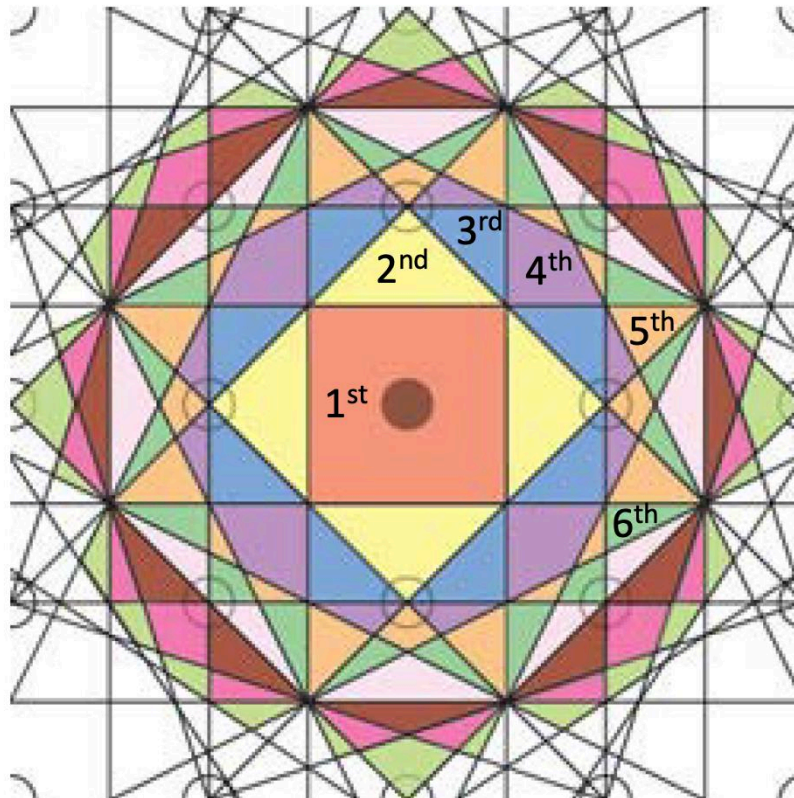
- 1) Choose one reciprocal lattice point as the starting point;
- 2) Draw perpendicular bisecting planes (垂直平分面) to all the reciprocal lattice vectors from the starting point;
- 3) The reciprocal space is then divided into different **polyhedral (多面体) zones enclosing the starting point**;
- 4) These polyhedral zones are called **Brillouin zones**.

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The Brillouin zones of a 2D square lattice.

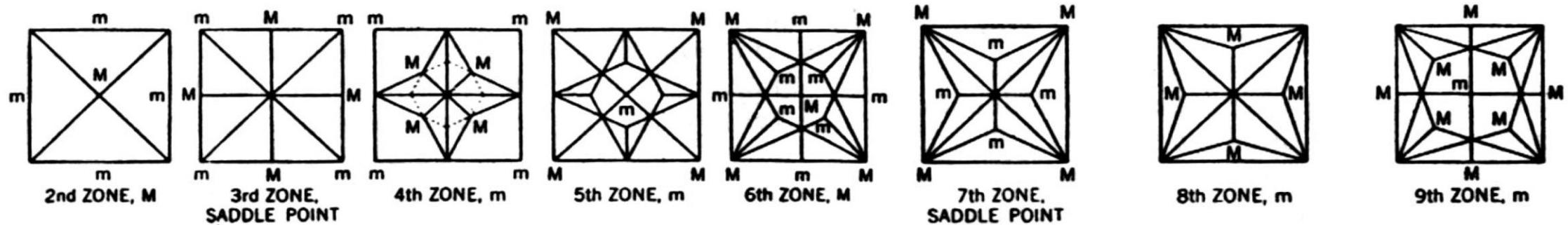


Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The Brillouin zones of a 2D square lattice.



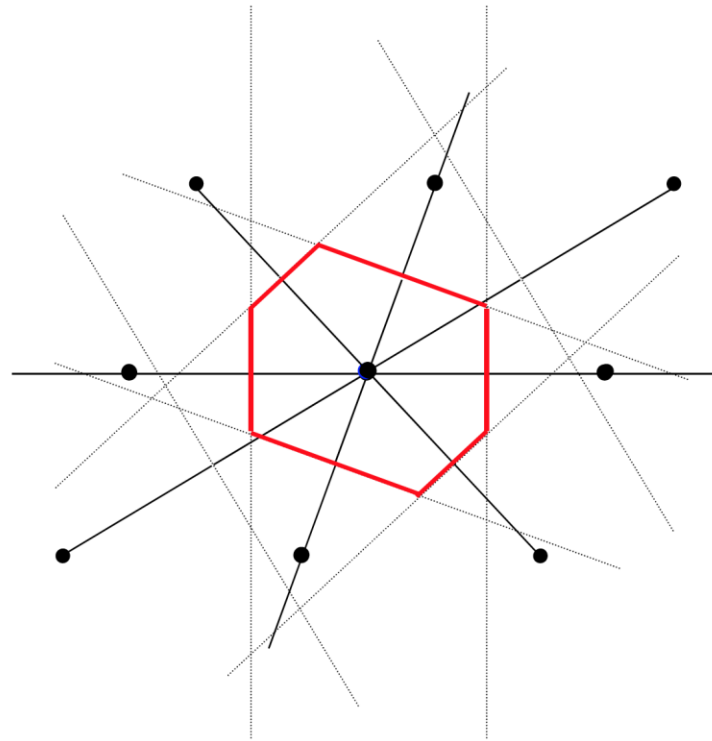
Reduction to the 1st zone for the second through ninth zones of the 2D square lattice.

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The **1st Brillouin zone** (第一布里渊区, 又称简约布里渊区) is defined as the **Wigner-Seitz primitive cell** of the reciprocal lattice.

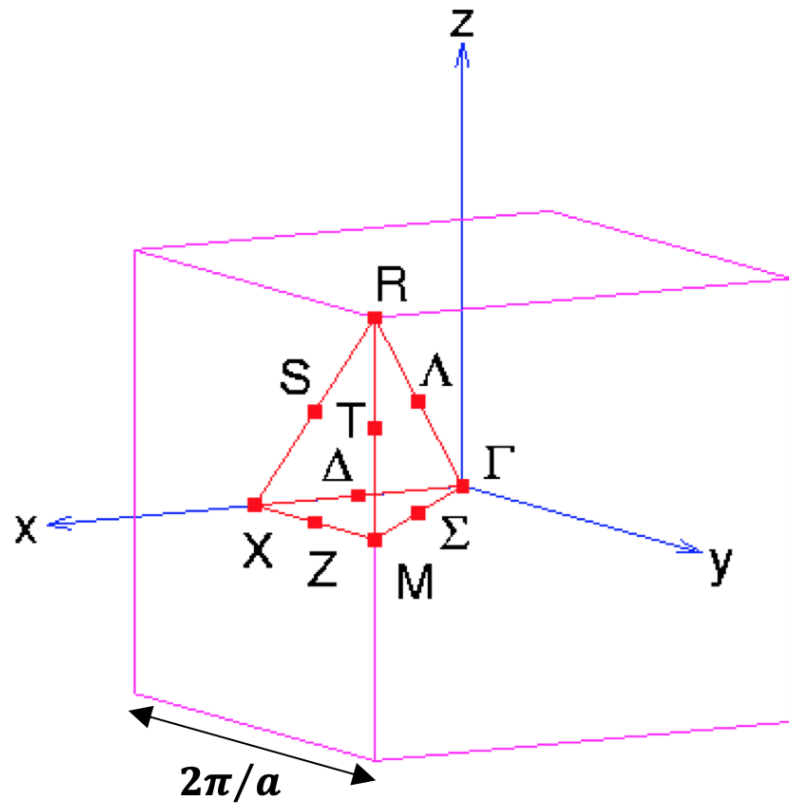


Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The 1st Brillouin zone of a *sc* lattice and the **points of high symmetry** (高对称点).



$$\Gamma: (0, 0, 0)$$

$$X: \frac{\pi}{a} (1, 0, 0)$$

$$R: \frac{\pi}{a} (1, 1, 1)$$

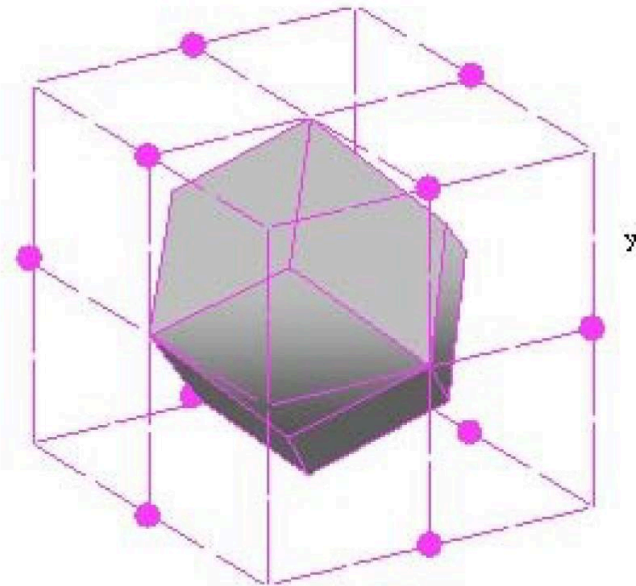
$$M: \frac{\pi}{a} (1, 1, 0)$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)

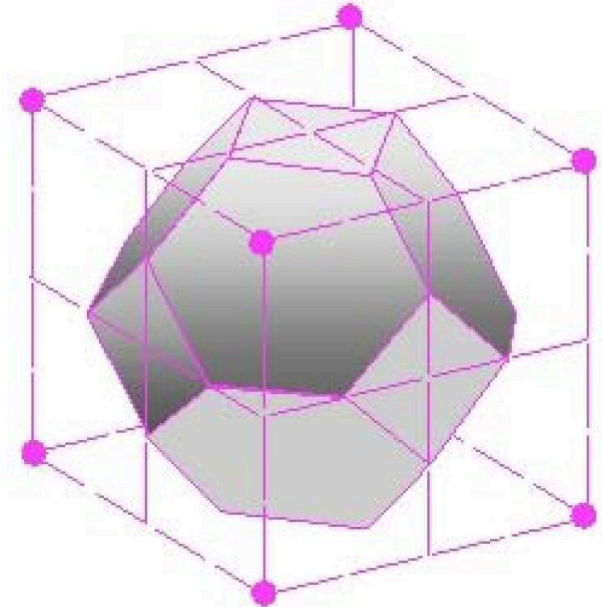


➤ Brillouin Zones (布里渊区)

❖ The WS cell and 1st Brillouin zone of a *fcc* lattice (*bcc* reciprocal lattice).



Wigner-Seitz Cell for
Face Centered Cubic Lattice



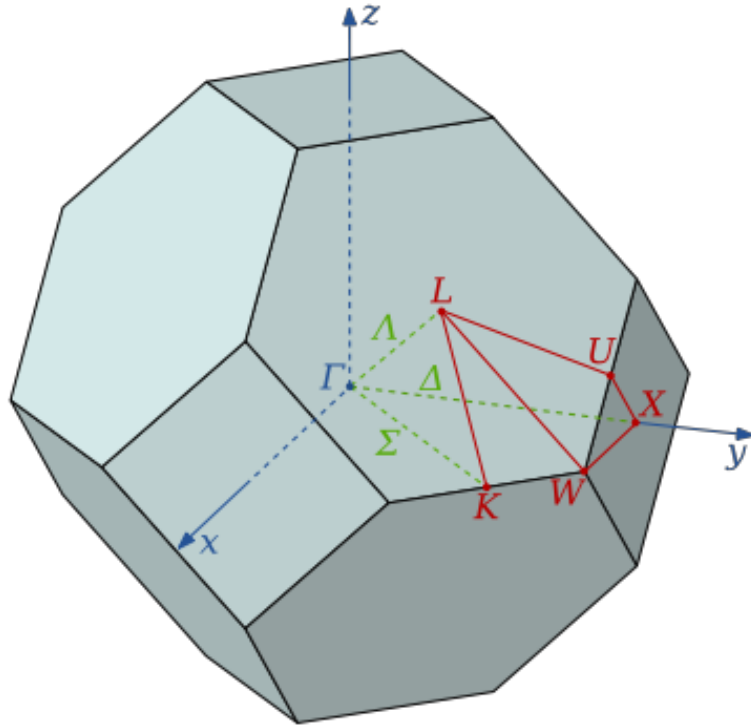
Brillouin Zone =
Wigner-Seitz Cell for
Reciprocal Lattice

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The 1st Brillouin zone of a *fcc* lattice (*bcc* reciprocal lattice) and the points of high symmetry.



$$\Gamma: (0, 0, 0)$$

$$X: \frac{2\pi}{a} (1, 0, 0)$$

$$L: \frac{2\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$$

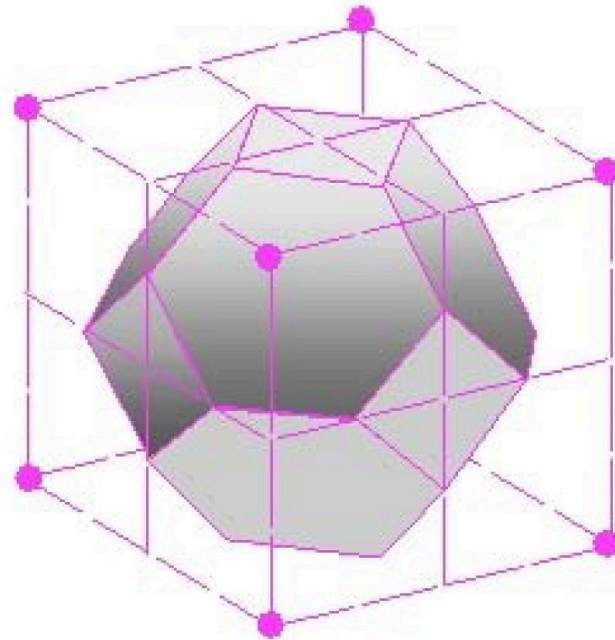
$$K: \frac{2\pi}{a} \left(\frac{3}{4}, \frac{3}{4}, 0 \right)$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)

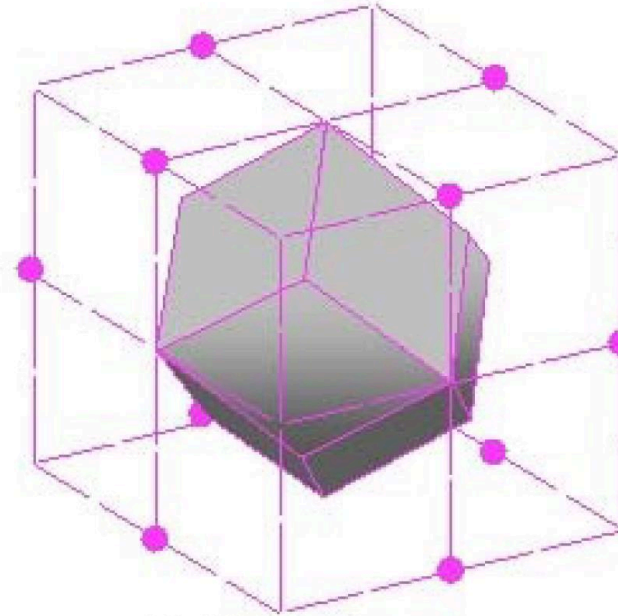


➤ Brillouin Zones (布里渊区)

❖ The WS cell and 1st Brillouin zone of a *bcc* lattice (*fcc* reciprocal lattice).



Wigner-Seitz Cell for
Body Centered Cubic Lattice



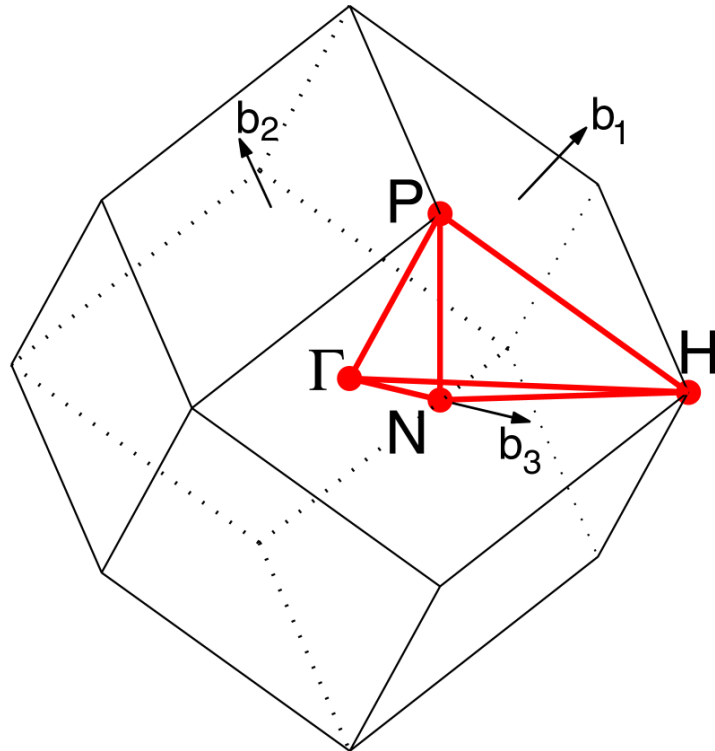
Brillouin Zone =
Wigner-Seitz Cell for
Reciprocal Lattice

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Brillouin Zones (布里渊区)

❖ The 1st Brillouin zone of a *bcc* lattice (*fcc* reciprocal lattice) and the points of high symmetry.



$$\Gamma: (0, 0, 0)$$

$$H: \frac{2\pi}{a} (1, 0, 0)$$

$$P: \frac{2\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right)$$

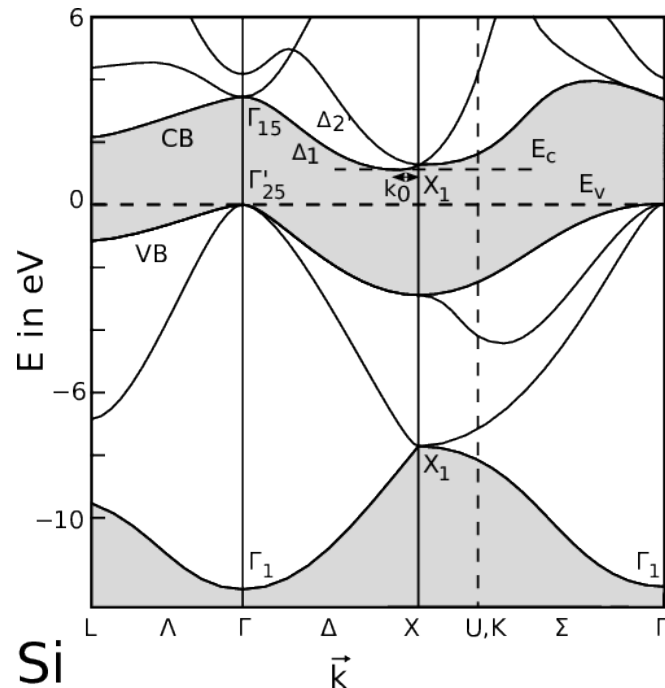
$$N: \frac{2\pi}{a} \left(\frac{1}{2}, \frac{1}{2}, 0 \right)$$

Chapter 1.4: Reciprocal Lattice (倒易点阵)

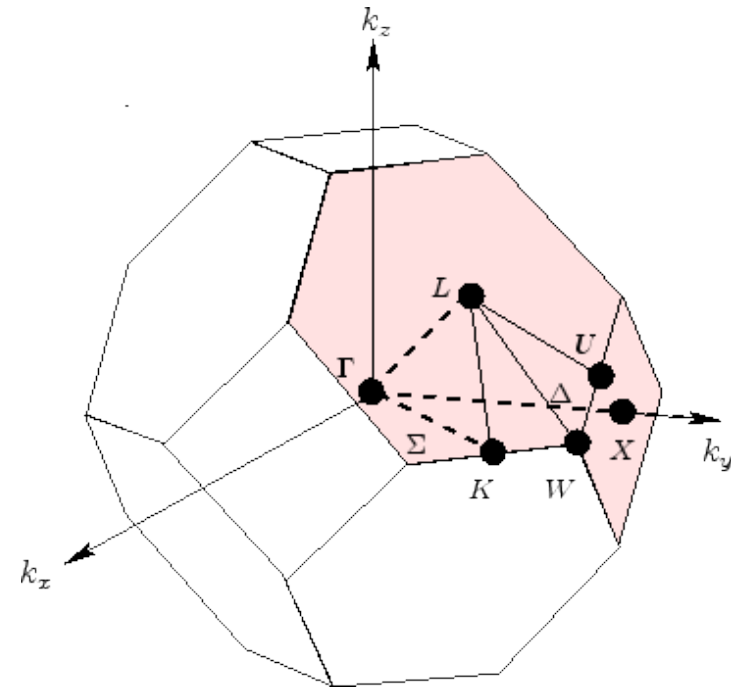


➤ Brillouin Zones (布里渊区)

❖ Band dispersion and the points of high symmetry.



Electron band dispersion of Si: $E_n(k)$, with k the lattice vector in reciprocal space and n the band index.



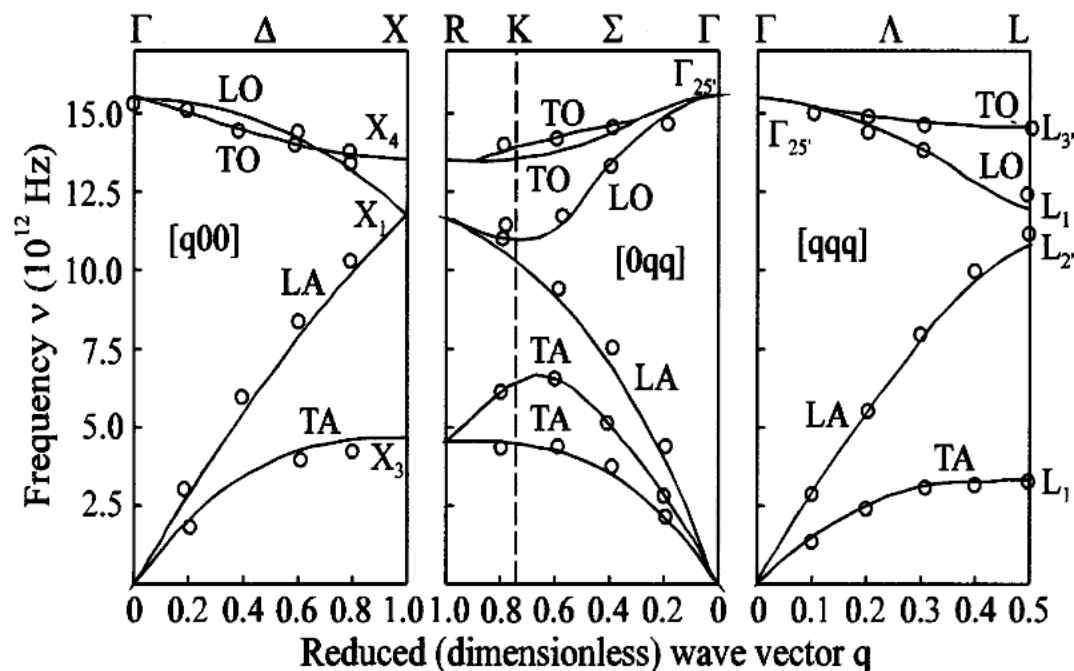
bcc reciprocal lattice

Chapter 1.4: Reciprocal Lattice (倒易点阵)

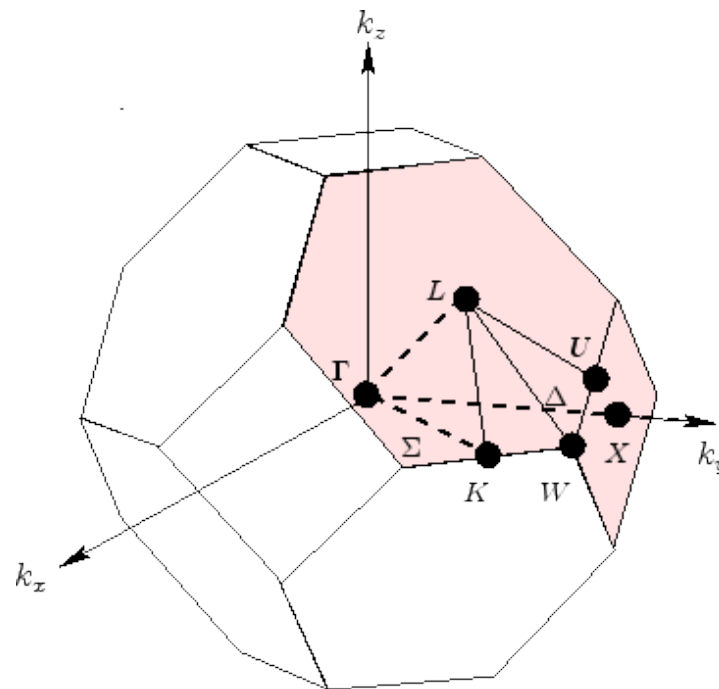


➤ Brillouin Zones (布里渊区)

❖ Band dispersion and the points of high symmetry.



Phonon band dispersion of Si: with q the lattice vector in reciprocal space.



bcc reciprocal lattice



Summary (总结)

Chapter 1.4: Reciprocal Lattice (倒易点阵)



➤ Summary (总结)

❖ Reciprocal lattices.

❖ Connection between reciprocal and direct lattices: **6**

❖ Typical reciprocal lattices:

<i>sc</i> lattice	↔	<i>sc</i> lattice
<i>fcc</i> lattice	↔	<i>bcc</i> lattice
<i>bcc</i> lattice	↔	<i>fcc</i> lattice

❖ Brillouin zones.



试证明:

倒格子矢量 $G = h_1 b_1 + h_2 b_2 + h_3 b_3$ 垂直于密勒指数为 $(h_1 h_2 h_3)$ 的晶面系。

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