Fundamentals of Solid State Physics

The Reciprocal Lattice
倒易点阵

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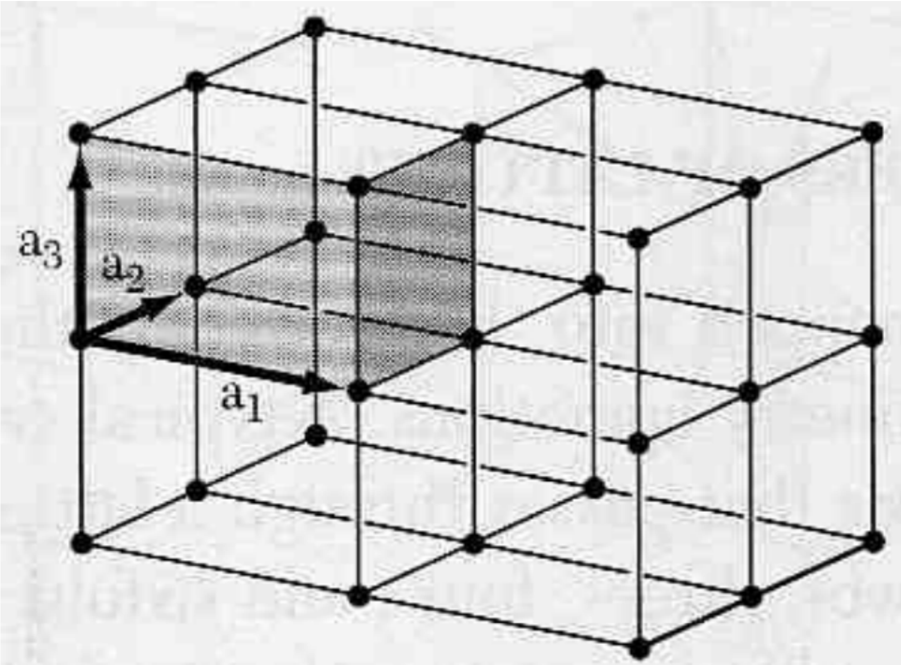
Bravais Lattice 布拉菲点阵

- Each point is *exactly* the same
- Position of each point

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

***n*$_1$, *n*$_2$, *n*$_3$ cover *all* the integers**

- (a_1, a_2, a_3) primitive vectors 基矢量



Real Space
正空间

Direct Lattice
正点阵 / 正格子

Lattice

- Certain physical properties *F*(r) in the crystal
  - electron density, electrical field, ...

- If *F*(r) is a periodic function

$$F(\mathbf{r}) = F(\mathbf{r} + \mathbf{R})$$

$$\rightarrow \quad F(\mathbf{r}) = \sum_{\mathbf{G}} F_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$$

Fourier expansion

$$\rightarrow \quad \exp(i\mathbf{G} \cdot \mathbf{R}) = 1$$

Reciprocal Lattice 倒易点阵

$$\exp(i\mathbf{G}\cdot\mathbf{R})=1$$

- For a Bravais lattice

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

n_1, n_2, n_3 are integers

- We define vector G as

$$\mathbf{G}=m_1\mathbf{b}_1+m_2\mathbf{b}_2+m_3\mathbf{b}_3$$

m_1, m_2, m_3 are integers

(b_1, b_2, b_3) forms reciprocal lattice (倒易点阵 / 倒格子)
G is in the reciprocal space (倒易空间 / 倒空间)

Reciprocal Lattice 倒易点阵

$$\exp(i\mathbf{G}\cdot\mathbf{R})=1 \rightarrow \mathbf{G}\cdot\mathbf{R}=2\pi\cdot N$$

- **One solution**

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

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

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

Reciprocal Lattice 倒易点阵

$$\exp(i\mathbf{G}\cdot\mathbf{R})=1 \rightarrow \mathbf{G}\cdot\mathbf{R}=2\pi\cdot N$$

- One can have

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

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

(b_1, b_2, b_3) is primitive vectors to form reciprocal lattice (also a Bravais lattice)

The reciprocal lattice is the Fourier transform of the direct lattice

Reciprocal Lattice 倒易点阵

- The reciprocal lattice of a Bravais lattice is also a Bravais lattice
- The reciprocal lattice of a reciprocal lattice is the original lattice
- The primitive cell volume of the reciprocal lattice

$$V_{\mathbf{G}} = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{V_{\mathbf{R}}}$$

$$V_{\mathbf{R}} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$ is the volume of the original cell

Reciprocal Lattice 倒易点阵

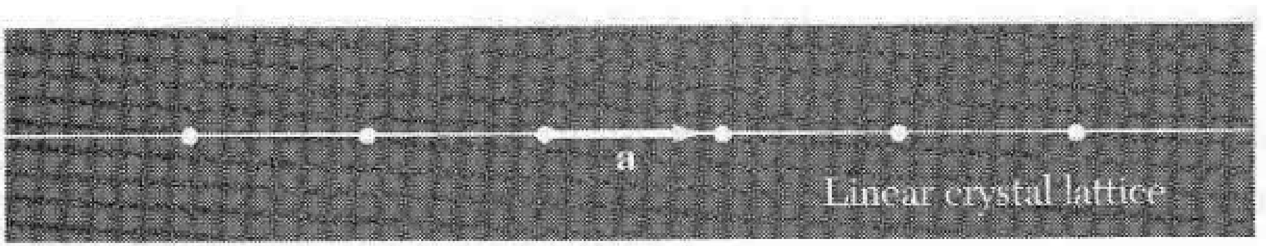
- 1D lattice
- 2D lattice
- Simple Cubic (SC)
- BCC
- FCC

1D Lattice

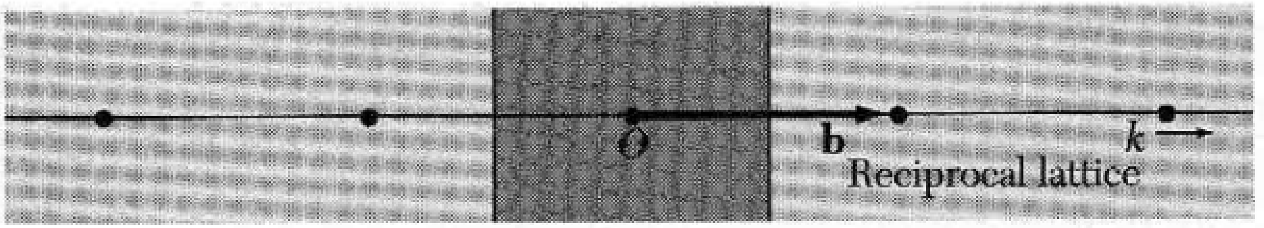
$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

$$\mathbf{a} = a\hat{\mathbf{x}}$$

$$\rightarrow \quad \mathbf{b} = \frac{2\pi}{a}\hat{\mathbf{x}}$$



real space



reciprocal space

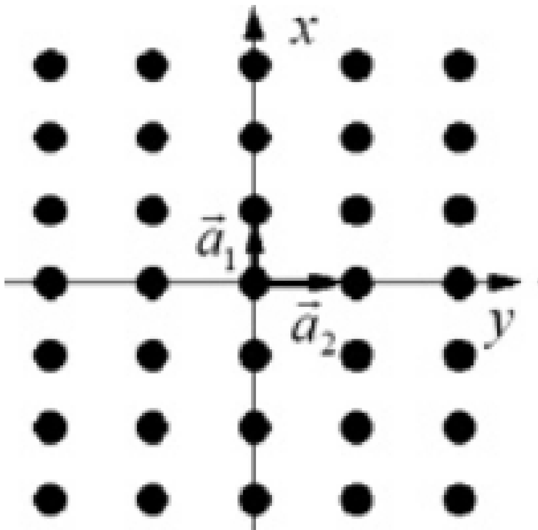
2D Rectangular Lattice

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

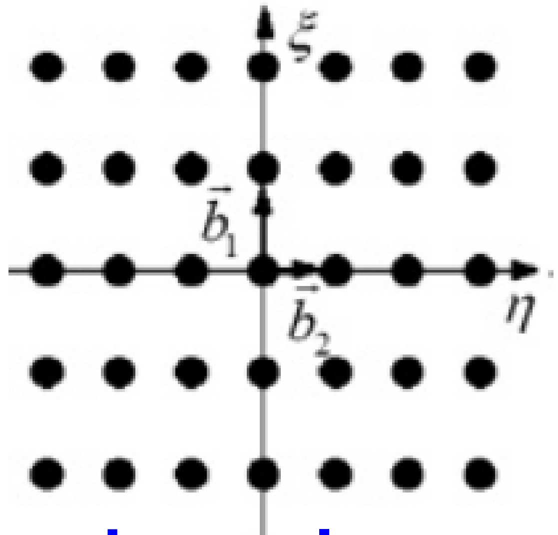
$$\mathbf{a}_1 = a_1\hat{\mathbf{x}}$$
$$\mathbf{a}_2 = a_2\hat{\mathbf{y}}$$

→

$$\mathbf{b}_1 = \frac{2\pi}{a_1}\hat{\mathbf{x}}$$
$$\mathbf{b}_2 = \frac{2\pi}{a_2}\hat{\mathbf{y}}$$



→



real space

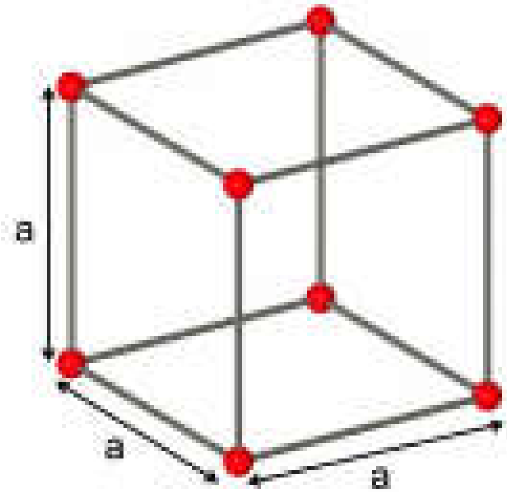
reciprocal space

Simple Cubic (SC)

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

→

$$\mathbf{b}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}$$
$$\mathbf{b}_2 = \frac{2\pi}{a}\hat{\mathbf{y}}$$
$$\mathbf{b}_2 = \frac{2\pi}{a}\hat{\mathbf{z}}$$



direct lattice

the reciprocal lattice is still SC

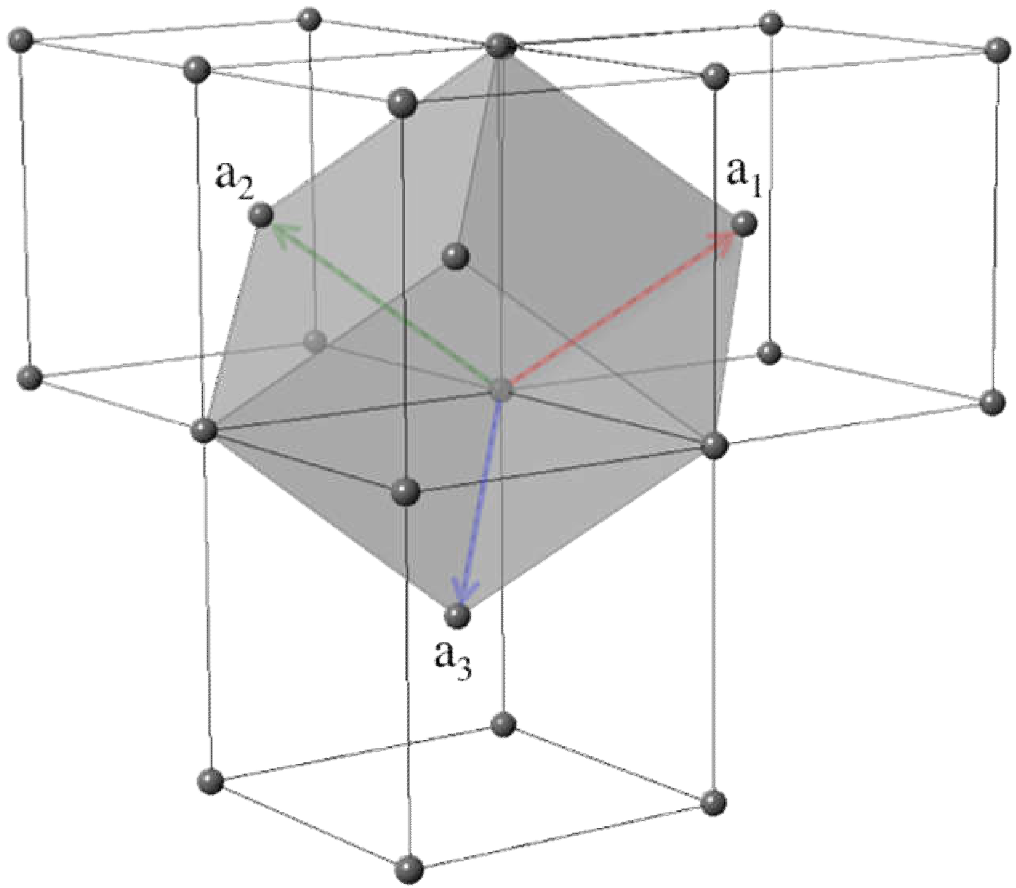
BCC

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

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

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

primitive cell



BCC

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

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

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

→

$$\mathbf{b}_1 = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{y}} + \hat{\mathbf{z}}\right)$$

$$\mathbf{b}_2 = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{z}} + \hat{\mathbf{x}}\right)$$

$$\mathbf{b}_3 = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{x}} + \hat{\mathbf{y}}\right)$$

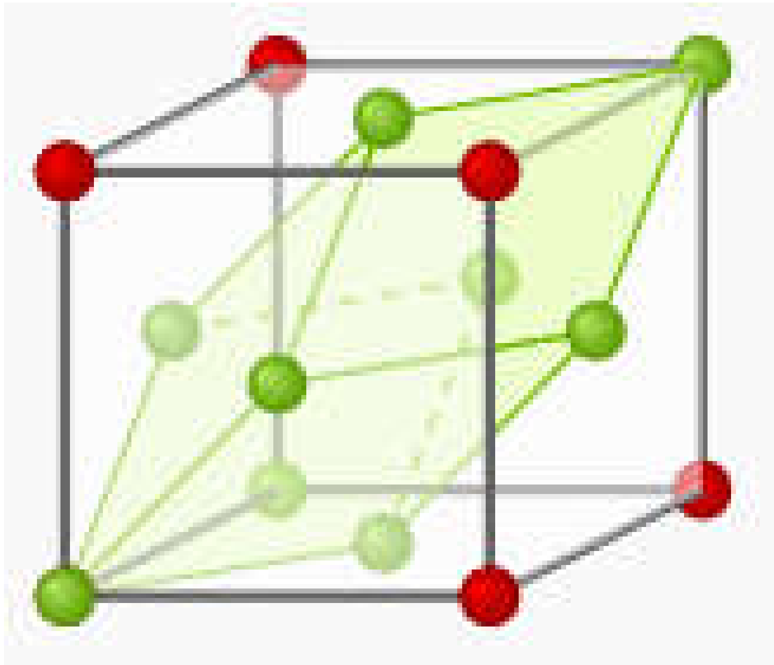
FCC

primitive cell

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

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

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



FCC

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

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

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

→

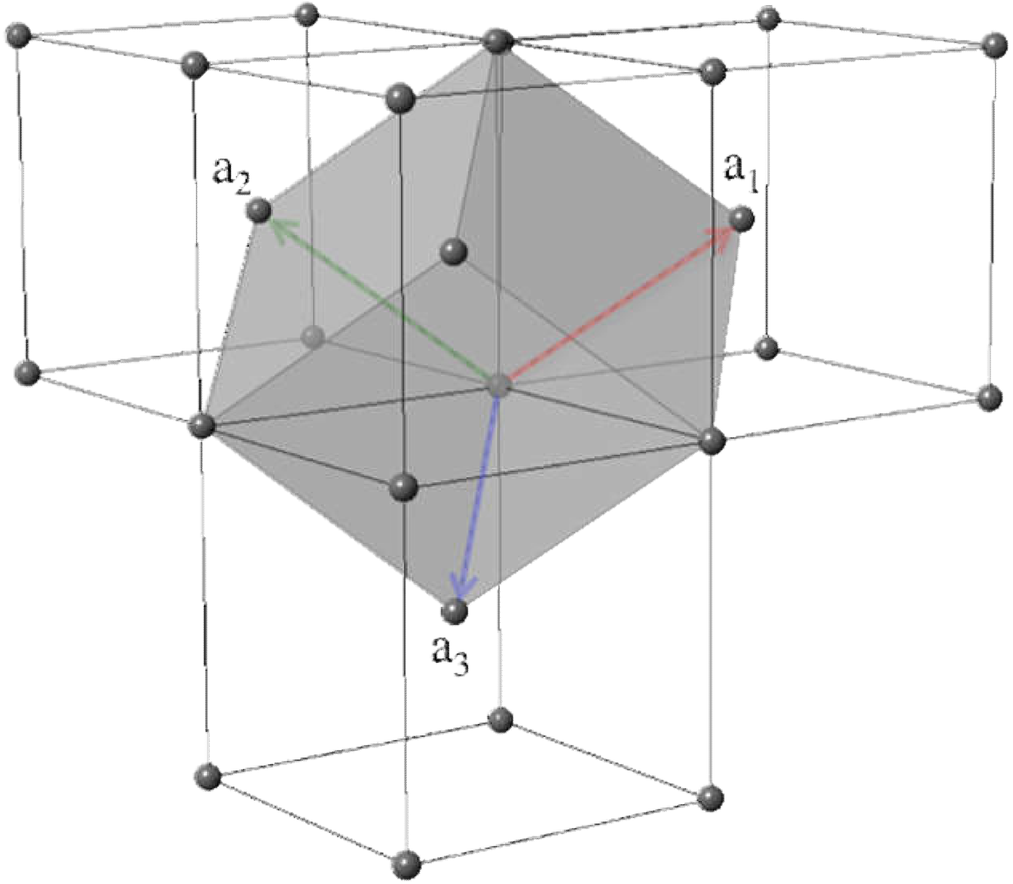
$$\mathbf{b}_1 = \frac{4\pi}{a}\frac{1}{2}\left(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}\right)$$

$$\mathbf{b}_2 = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}\right)$$

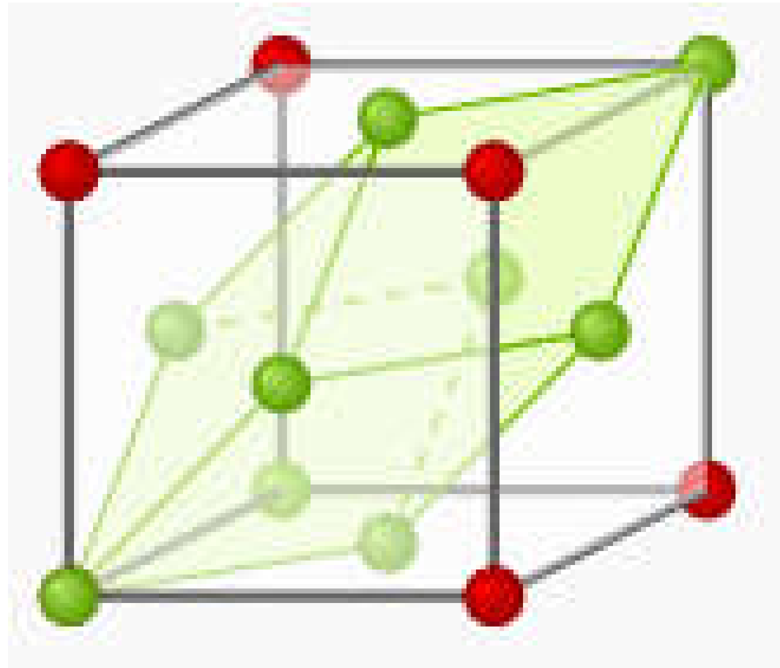
$$\mathbf{b}_3 = \frac{4\pi}{a}\frac{1}{2}\left(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}\right)$$

BCC and FCC

BCC



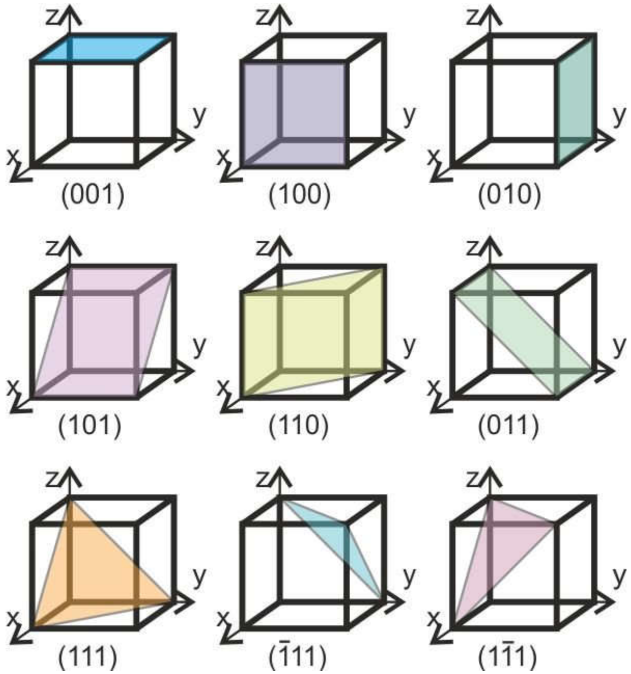
FCC



The reciprocal lattice of BCC is FCC
The reciprocal lattice of FCC is BCC

Miller Indices - Plane 晶面

- crystal plane (*hkl*)
  - intercepts at (a_1/h, a_2/k, a_3/l)



For all Bravais lattices, not only cubic we have:

1. The (*hkl*) plane ⊥ reciprocal lattice vector G

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

2. The interplanar distance of (hkl) plane $d_{(hkl)}$

$$d_{(hkl)} = \frac{2\pi}{|\mathbf{G}|}$$

Brillouin Zones 布里渊区

- The *First Brillouin Zone (FBZ)*
  - **the Wigner-Seitz cell of the reciprocal lattice**

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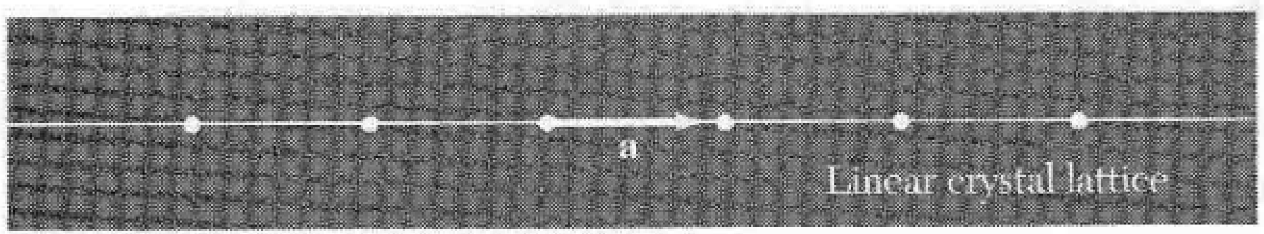
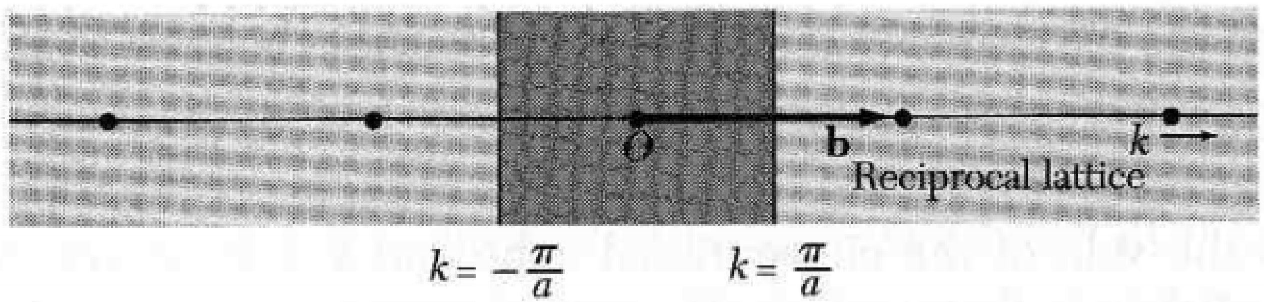


real space



reciprocal space

1D lattice, FBZ

$$-\frac{\pi}{a} < k < \frac{\pi}{a}$$

Brillouin Zones 布里渊区

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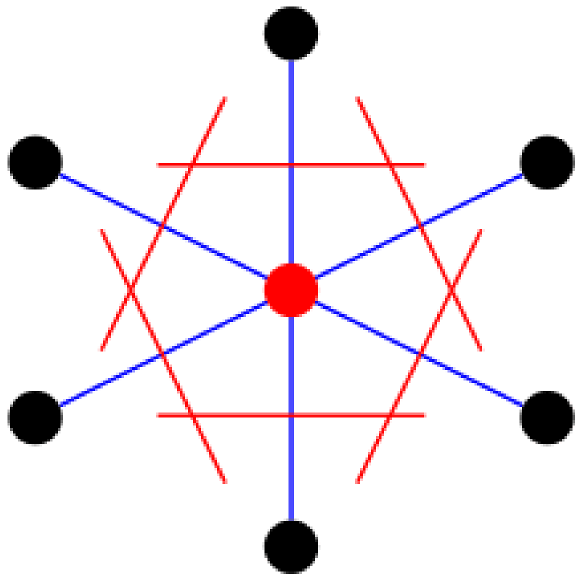
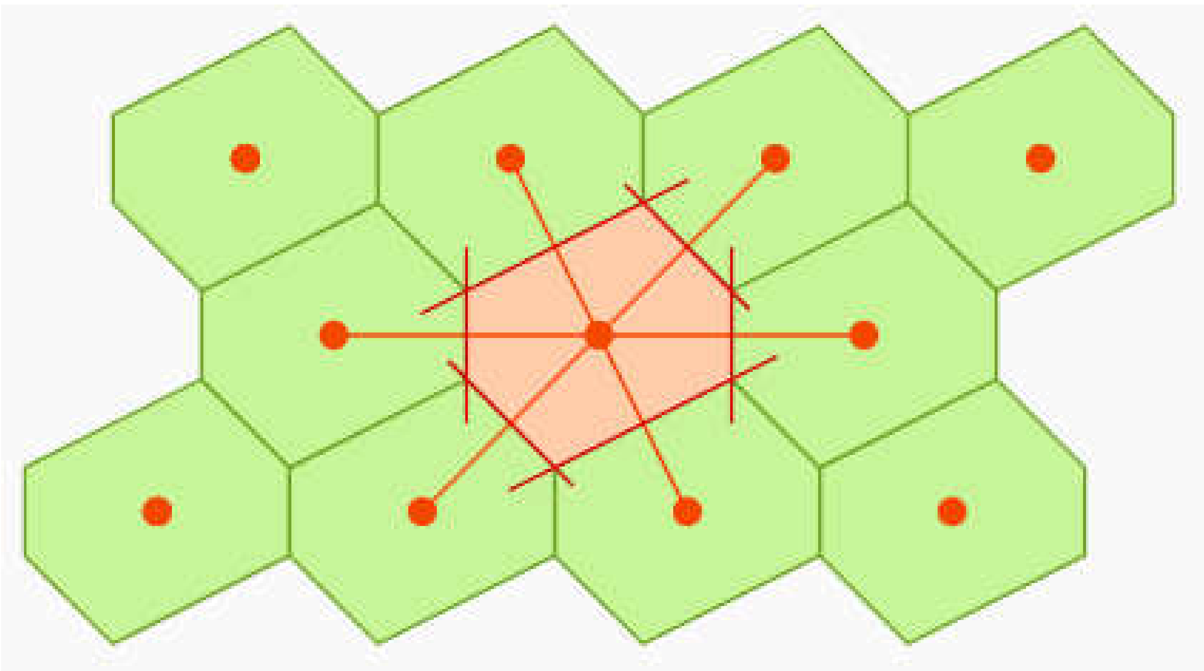
  - the Wigner-Seitz cell of the reciprocal lattice





2D lattice

Brillouin Zones 布里渊区

- The *First Brillouin Zone (FBZ)*
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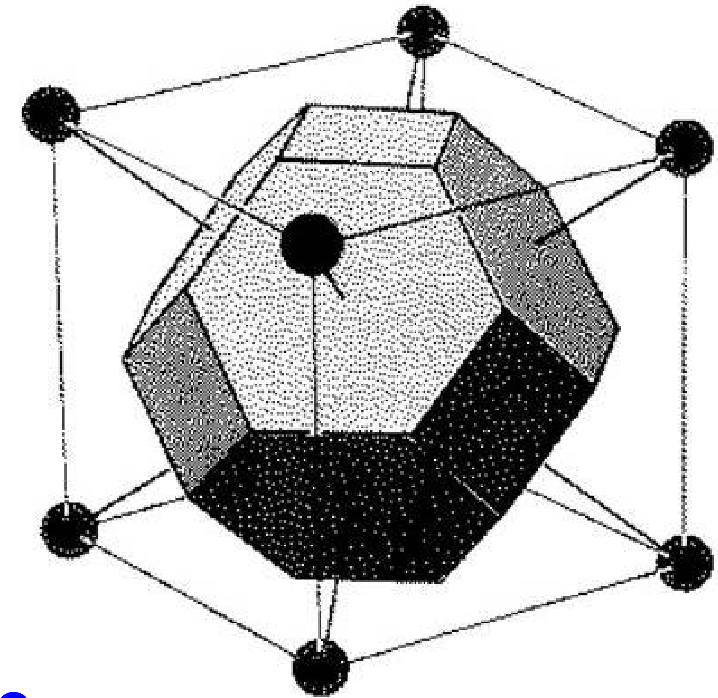
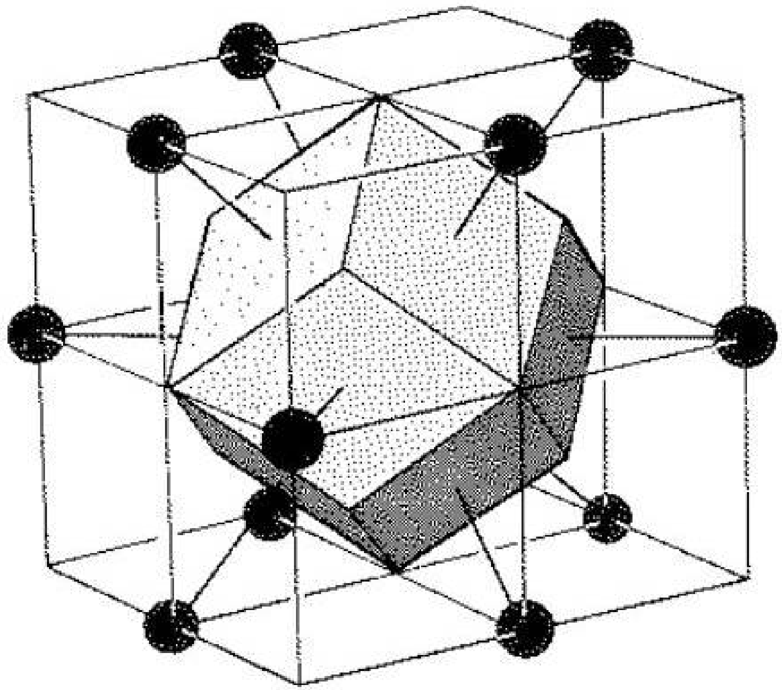
3D lattice



BCC

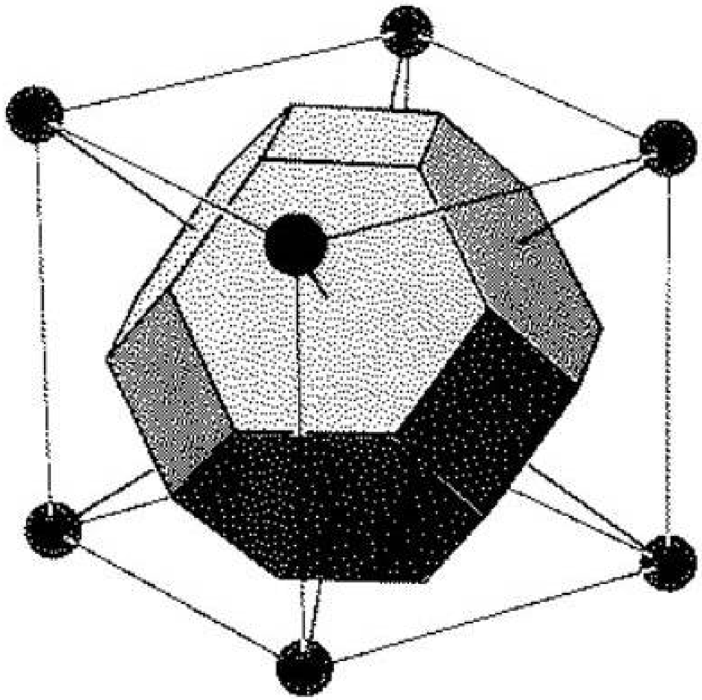


FCC

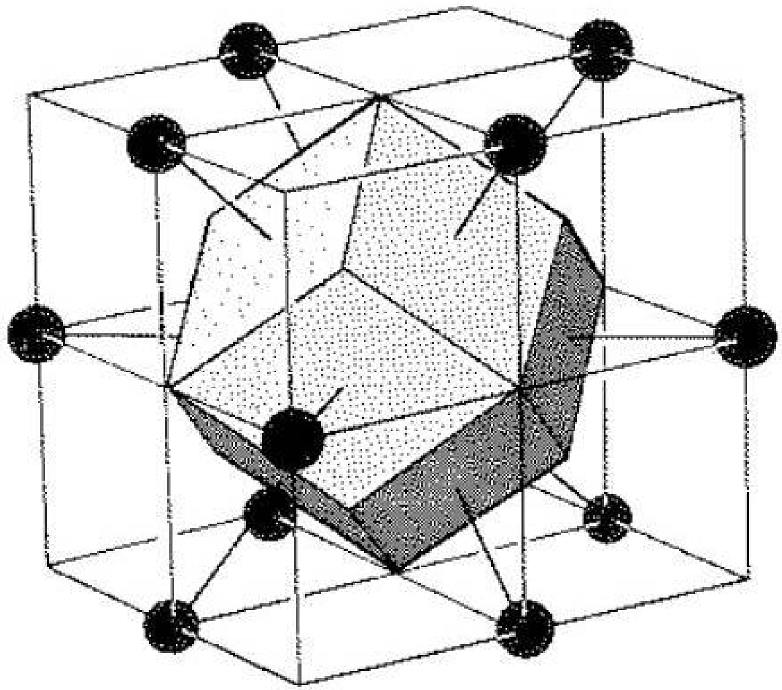
Wigner-Seitz Cell

Brillouin Zones 布里渊区

- The *First Brillouin Zone (FBZ)*
  - the Wigner-Seitz cell of the reciprocal lattice



FBZ for FCC



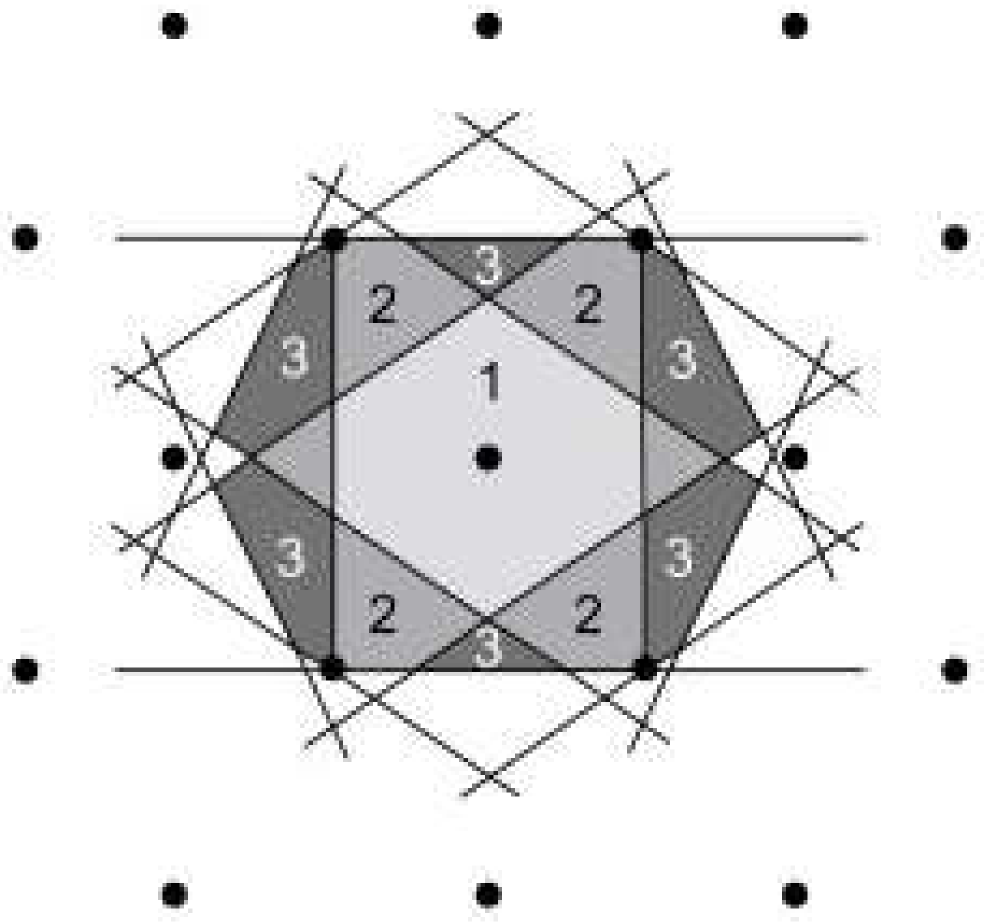
FBZ for BCC

Q: What is the volume of the FBZ?

Brillouin Zones 布里渊区

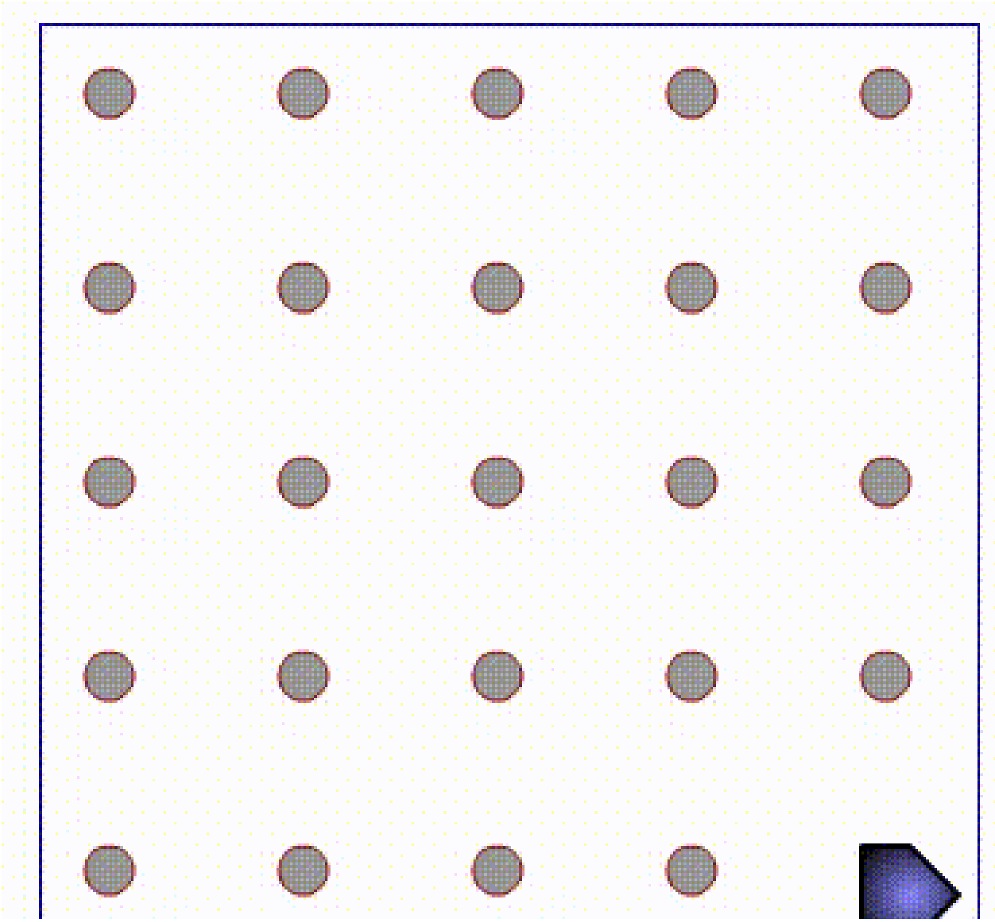
- Higher-order Brillouin Zones (BZs)
  - 2nd BZ
  - 3rd BZ
  - ...

All the Brillouin Zones have the same area / volume.



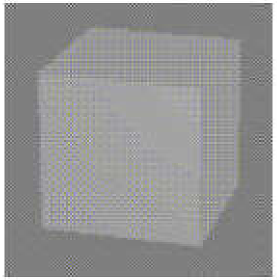
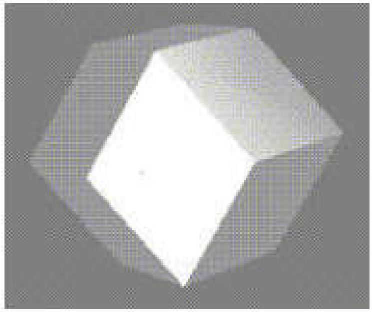
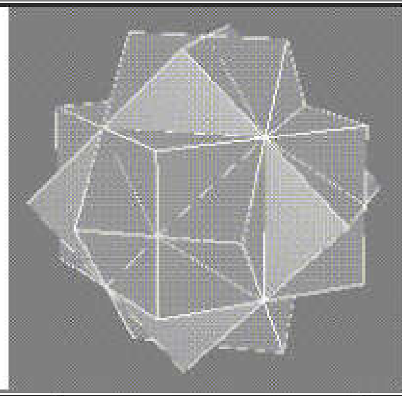
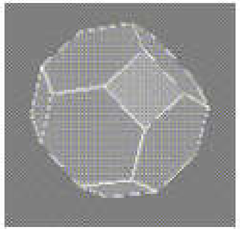
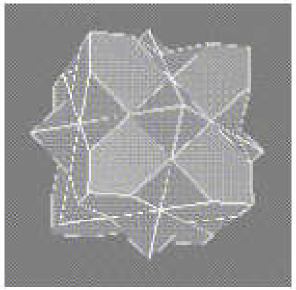
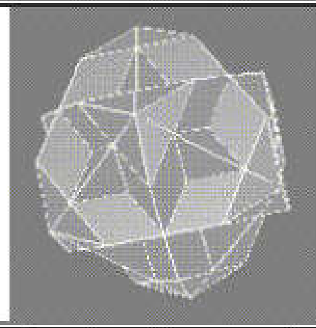
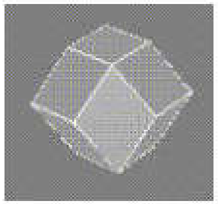
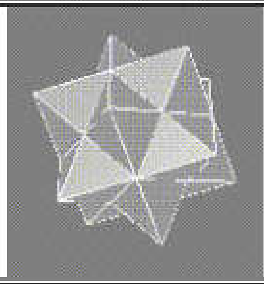
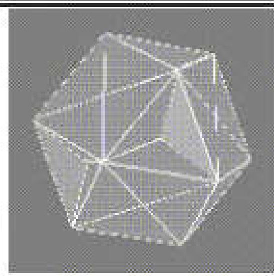
Brillouin Zones 布里渊区

- **Higher-order Brillouin Zones (BZs)**
  - **2nd BZ**
  - **3rd BZ**
  - **...**



All the Brillouin Zones have the same area / volume.

Brillouin Zones 布里渊区

	First zone	Second zone	Third zone
SC			
FCC			
BCC			

All the Brillouin Zones have the same volume.

Thank you for your attention