

半导体及其分类

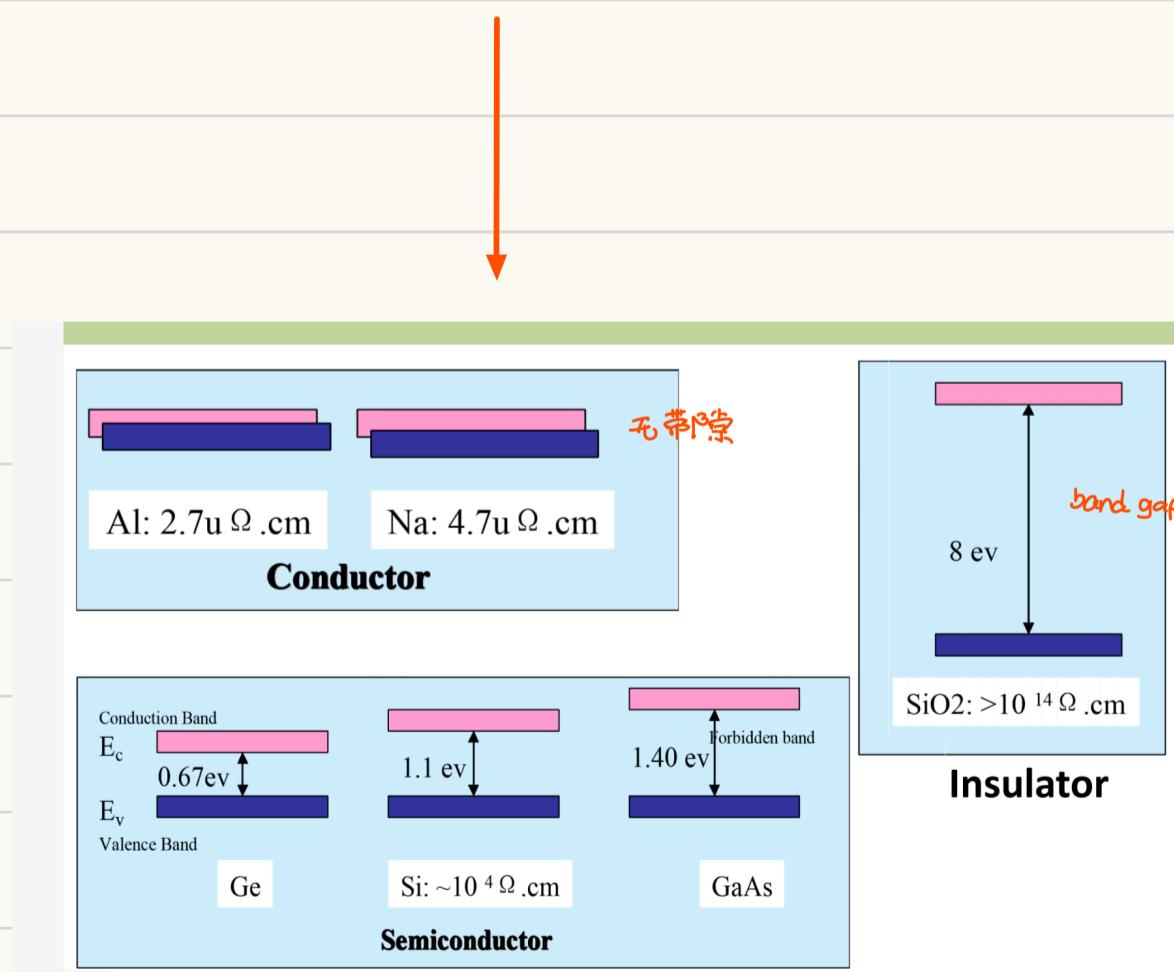
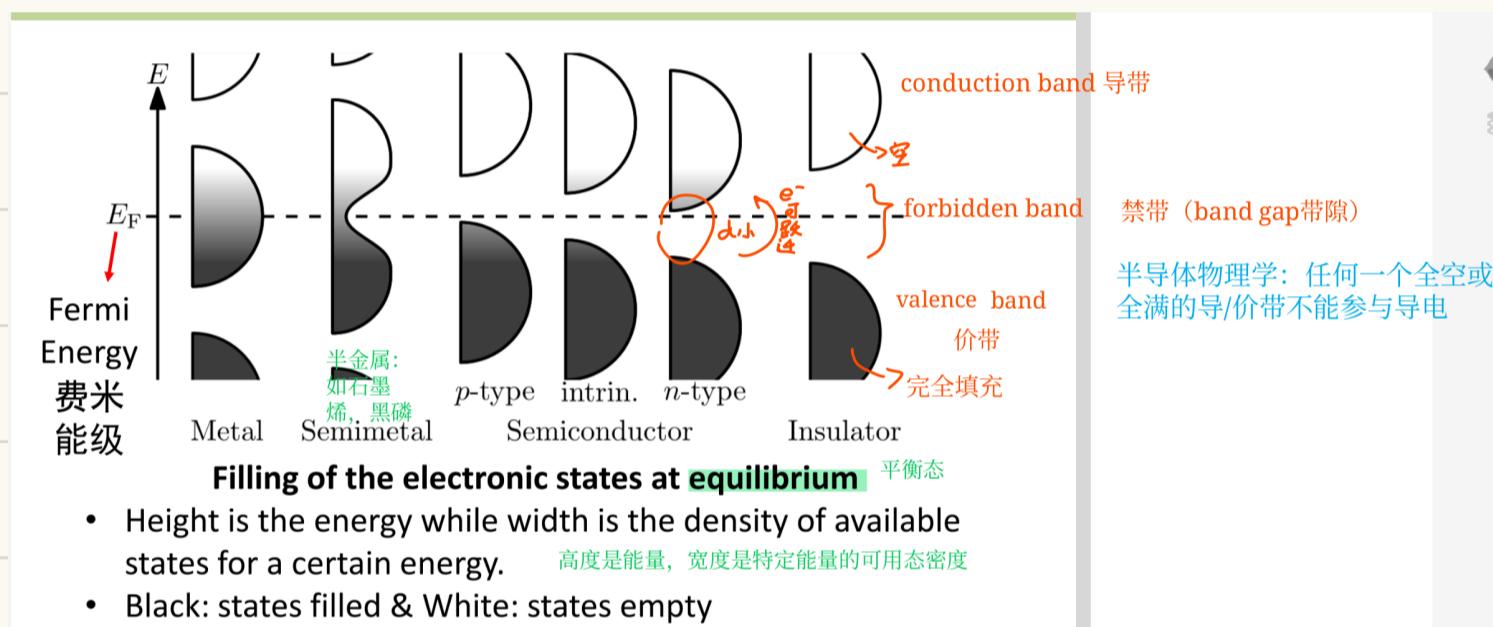
半导体定义问题

电阻率定义

- Low resistivity => "conductor": $\rho = 10^{-5} - 10^{-6} \Omega \cdot cm$
- High resistivity => "insulator": $\rho = 10^{14} - 10^{18} \Omega \cdot cm$
- Intermediate resistivity => "semiconductor": $\rho = 10^{-3} - 10^3 \Omega \cdot cm$
中级的

$$\tau \uparrow \quad \rho_{\text{semi}} \downarrow$$

能带结构



半导体的性质

- 可变电导率
- **Variable electrical conductivity:** The carrier density can be tuned by adding charged particles (doping) or applying an electric field (gating). 带电粒子 捆杂 $\sigma = \sigma_0 n^{1+\alpha}$
- **Heterojunction (异质结):** Two differently doped semiconducting materials are joined together, which is the basis of diodes, transistors and all modern electronics. 晶体管 现代电子器件 二极管
- **Excited electrons:** The injected energy (e.g. photon) creates a non-equilibrium situation, generating high energy charge carriers. (Solar cells, light-emitting diodes, fluorescent quantum dots, etc.) 激发电子 注入的能量 光子 非平衡状态 高能电荷载流子 太阳能电池 发光二极管 荧光量子点 热学的
- **Thermal conductivity and thermo-power:** For heat dissipation and thermoelectric generators etc. 散热 热电发电机

传统半导体

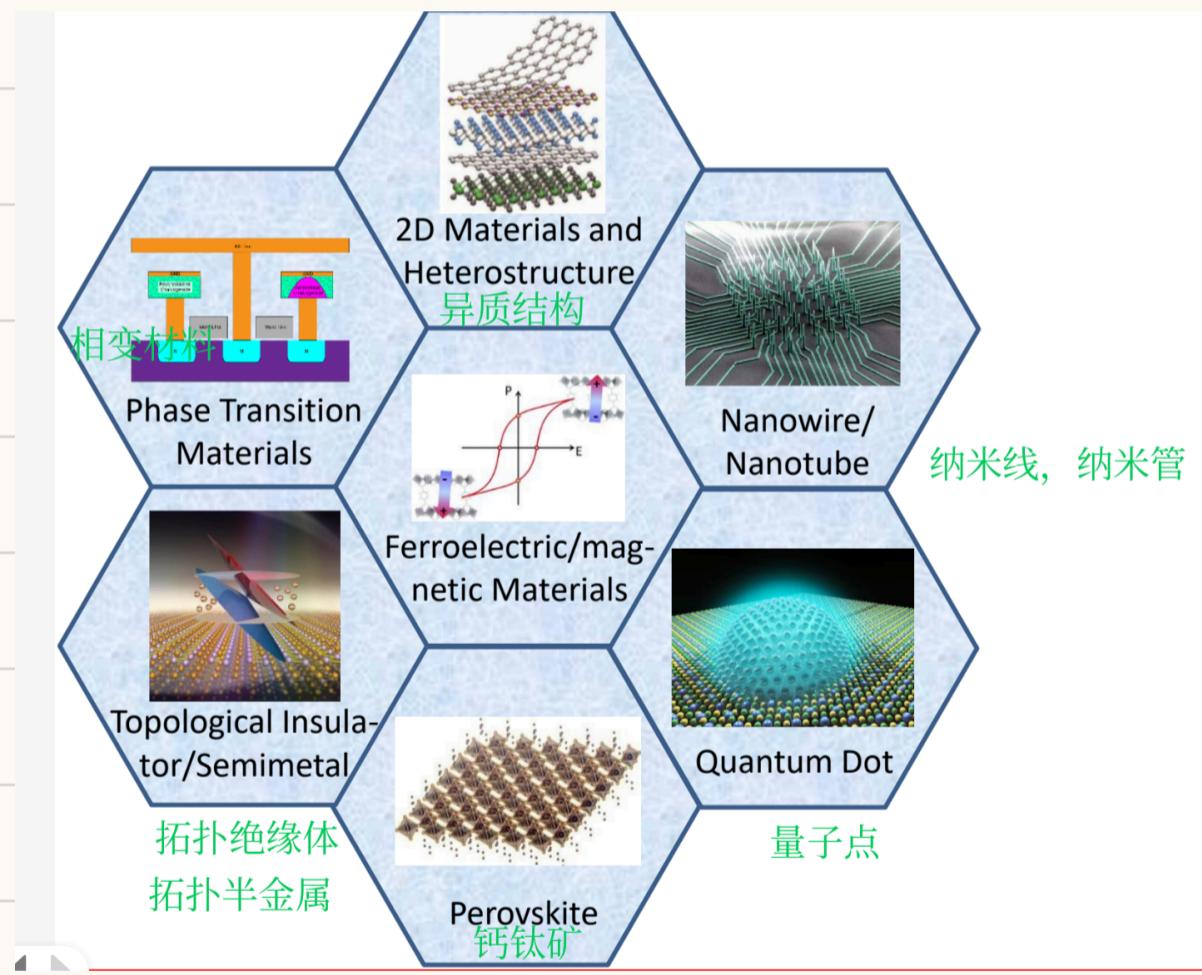
Traditional Semiconductor Materials

Elemental Semiconductors		IV Compound Semiconductors	
Si	Silicon	SiC	Silicon carbide
Ge	Germanium	SiGe	Silicon germanium
Binary III-V Compounds		Binary II-VI Compounds	
AlAs	Aluminum arsenide	CdS	Cadmium sulfide
AlP	Aluminum phosphide	CdTe	Cadmium telluride
AlSb	Aluminum antimonide	HgS	Mercury sulfide
GaAs	Gallium arsenide	ZnS	Zinc sulfide
GaP	Gallium phosphide	ZnTe	Zinc telluride
GaSb	Gallium antimonide		
InAs	Indium arsenide		
InP	Indium phosphide		
三元		四元	
Ternary Compounds		Quaternary Compounds	
Al _x Ga _{1-x} As	Aluminum gallium arsenide	Al _x Ga _{1-x} As _y Sb _{1-y}	Aluminum gallium arsenic antimonide
GaAs _{1-x} P _x	Gallium arsenic phosphide	Ga _x In _{1-x} As _{1-y} P _y	Gallium indium arsenic phosphide

Traditional Semiconductor Applications

Elemental Semiconductors	Compound Semiconductors
<ul style="list-style-type: none">* Silicon (Si)<ul style="list-style-type: none">- Electronic Components<ul style="list-style-type: none">... Diode, Transistor, Microprocessor, DRAM- Light Detector<ul style="list-style-type: none">... IR, Nuclear radiation	<ul style="list-style-type: none">* III-V Compounds<ul style="list-style-type: none">- GaAs, GaP, InP, InSb, GaN <small>光子</small>- Photonic devices<ul style="list-style-type: none">... LED, LD, PD- High speed, Low noise, High power electronics* II-VI Compounds <small>荧光</small><ul style="list-style-type: none">- Fluorescent screen<ul style="list-style-type: none">... ZnS
<ul style="list-style-type: none">* Germanium (Ge)<ul style="list-style-type: none">- Light Detector<ul style="list-style-type: none">... IR, Nuclear radiation	

新型半导体

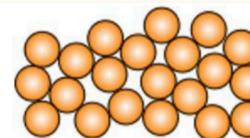


晶体结构

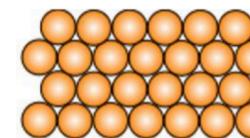
晶格：定义：构成晶体的原子在空间中的周期性排布。本质上就是空间点阵

➤ Amorphous materials (非晶)

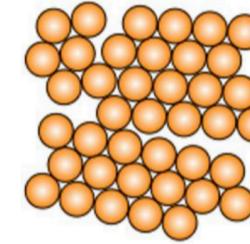
- Def.: Solid that lacks the long-range order.
- E.g.: Amorphous silicon (For solar cell, IR detection)



Amorphous



Single crystal



Polycrystalline

➤ Single crystal (单晶)

- Def.: Solid in which the crystal lattice of the entire sample is continuous and unbroken to the edges of the sample.
- E.g.: Silicon wafer, GaAs wafer (For IC chips)

➤ Polycrystalline materials (多晶)

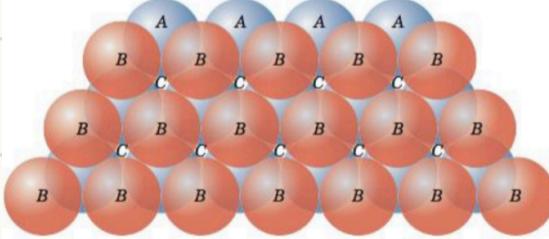
- Def.: Solid composed of many crystallites (微晶) of varying size and orientation.
- E.g.: Poly-silicon (For MOSFETs, large-scale photovoltaics)

Crystalline materials

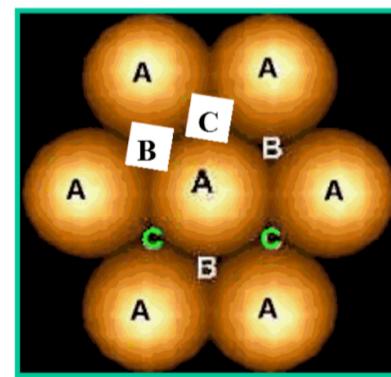
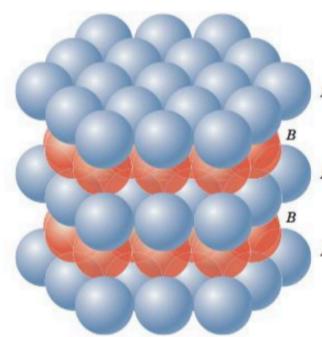
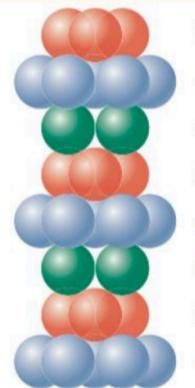
体心立方

Body-Centred Cubic (BCC)

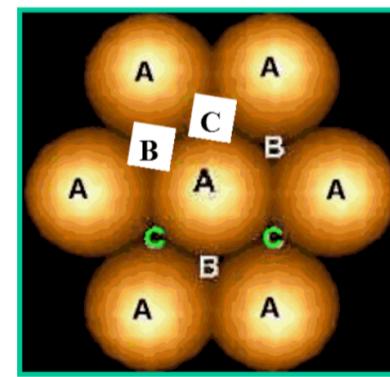
两种三维最密堆积



Three dimensional
close-packed structure



堆垛方式：
ABC ABC ABC...



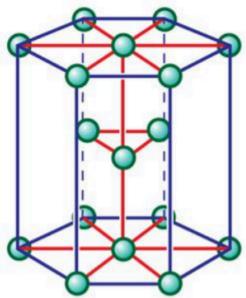
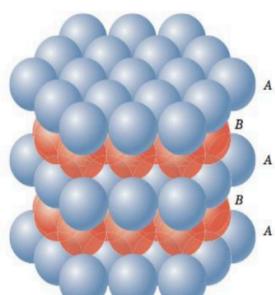
堆垛方式：
AB AB AB...

第三层与第一层重合方式相同(球心与A重合): 六方最密堆积

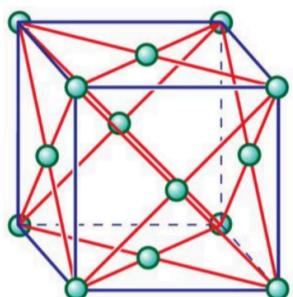
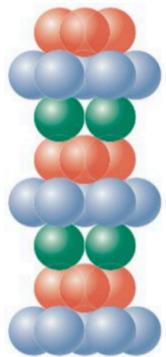
HCP结构

第三层与第一层重合方式不同(球心与C重合): 面心立方最密堆积

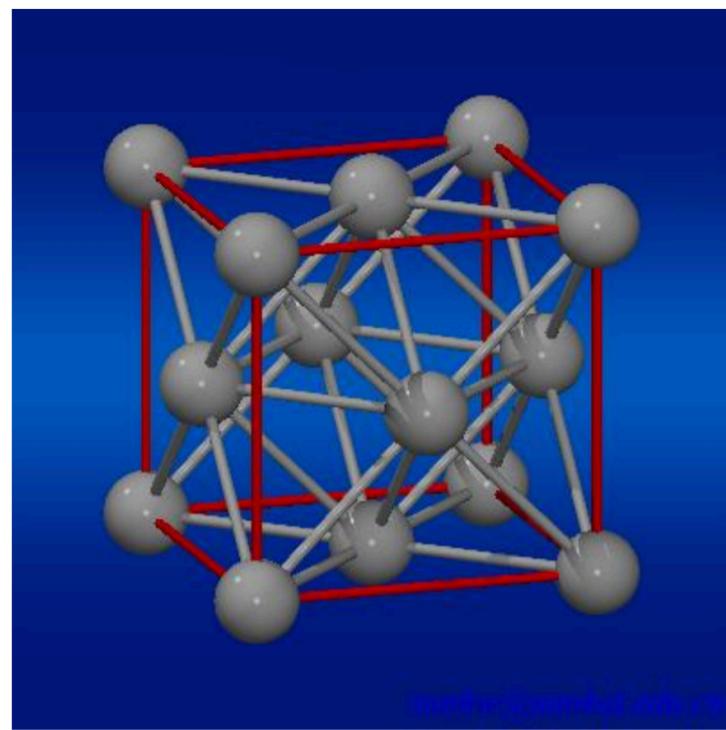
FCC结构



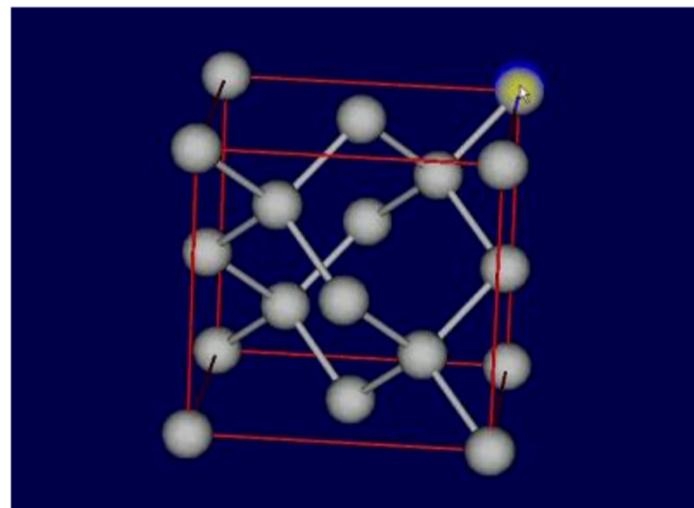
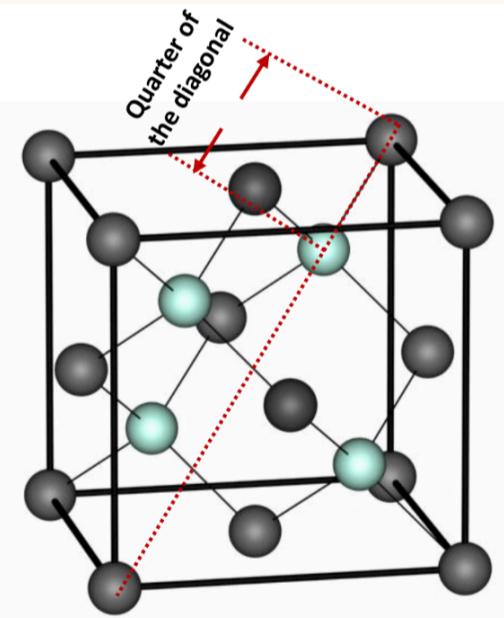
Hexagonal close packed crystal (HCP)
(六方密排晶体)



Face-centered cubic crystal (FCC)
(面心立方晶体)



金刚石晶格结构



- Diamond (金刚石) structure: Si, Ge
- Diamond-like crystal can be thought of as an FCC structure with four extra atoms placed at one quarter of the body diagonal of the cube.
- Each atom has 4 nearest neighbors.

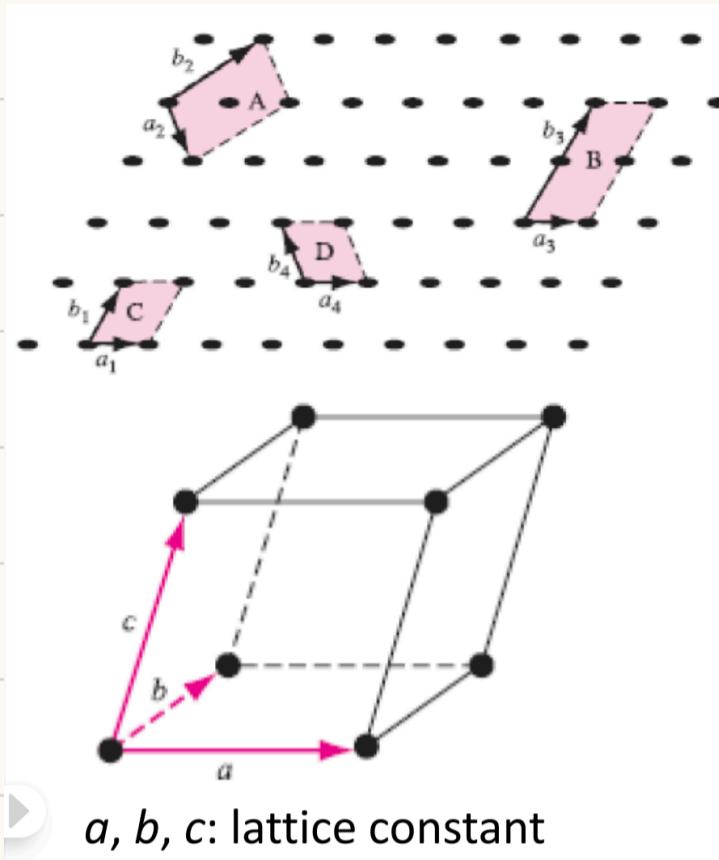
几种堆积方式对比

Lattice Parameters	Simple Cubic (SC)	Body Center Cubic (BCC)	Face Center Cubic (FCC)	Diamond
Cell edge length (a)	$2r$	$4r/\sqrt{3}$	$2\sqrt{2}r$	$8r/\sqrt{3}$
Atom Radius (r)	$a/2$	$\sqrt{3}/4a$	$\sqrt{2}/4a$	$\sqrt{3}/8a$
Coordination number (CN)	6	8	12	4
Number of atoms per unit cell	1	2	4	8
Atomic packing factor (APF)	$\pi/6 = 52\%$	$\pi\sqrt{3}/8 = 68\%$	$\pi\sqrt{2}/6 = 74\%$	$\pi\sqrt{3}/16 = 34\%$

六方最密堆积的APF也是74%

晶向与密勒指数

单胞与初基原胞



➤ A **unit cell** (单胞) is a small volume of the crystal that can be used to reproduce the entire crystal. (Macroscopic symmetry)

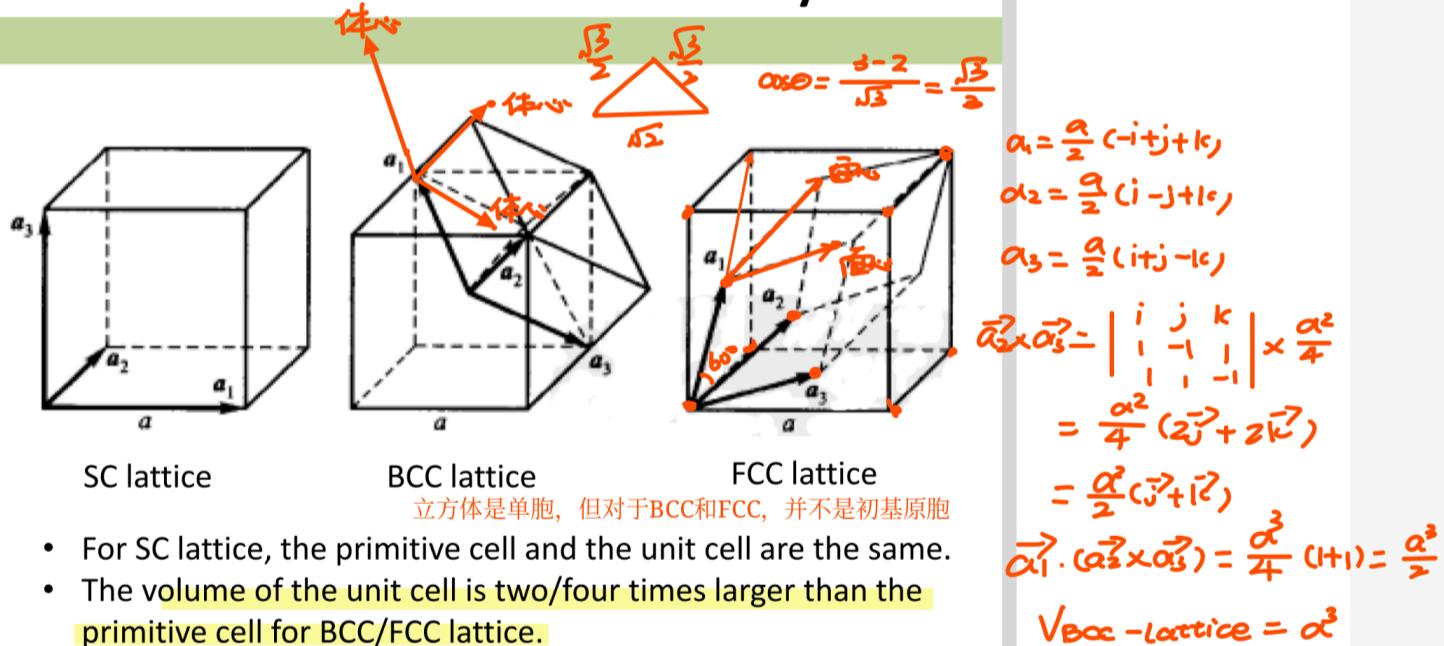
$$\vec{T}_m = m_1 \vec{a} + m_2 \vec{b} + m_3 \vec{c}$$

➤ A **primitive cell** (初基元胞) is the **smallest** unit cell that can be repeated to form the lattice. (Translational symmetry)

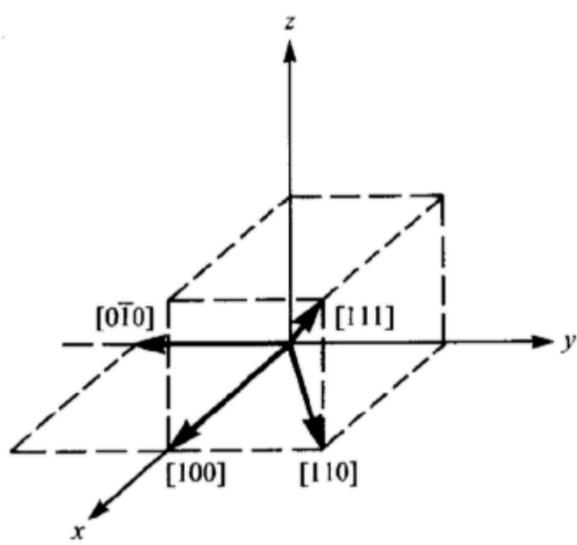
$$\vec{R}_I = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3$$

l_i is 整数

Primitive Cell and Unit Cell in a Crystal



由单胞构造初基原胞：三个非共面方向上寻找最近格点



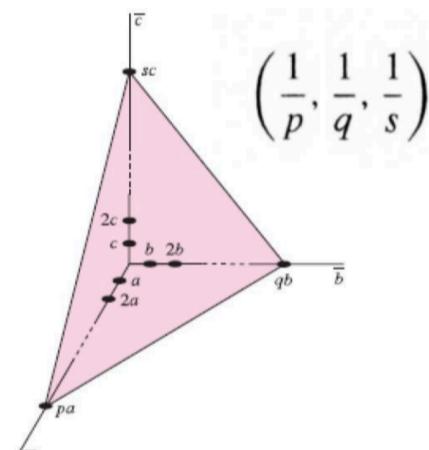
Sample direction vectors and the corresponding indices
样本方向向量和相应索引

- A particular direction in the crystal can be expressed as a set of three co-prime integers (互质整数) which are the components of a vector in the direction.

- Square brackets “[]” are used.
- The negative number is written as \bar{n} instead of $-n$
- 由于晶体对称性, 所有等效方向使用角括号
- Angle brackets are used for all equivalent directions by virtue of the crystal symmetry.

密勒指数

法向量, 互质整数



A crystal plane with intercepts to the axes
具有与轴截距的晶面

- The intercepts (截距) on the axes corresponds to pa , qb , and sc .
- Multiply by the lowest common denominator of $1/p$, $1/q$, and $1/s$.
乘以最小公分母
- Parentheses “(hkl)” are used.
- The negative number is written as \bar{n} instead of $-n$
- {hkl} are used for all equivalent directions by virtue of the crystal symmetry.

密勒指数标准求解步骤

➤ Step 1: Identify the intercepts on the x-, y- and z- axes.

Intercepts on the x-, y- and z-axes are at $x = \alpha$, $y = \beta$ and $z = \gamma$, respectively. If the surface is parallel to an axis, there would be no intercept on the axis. We shall consider the intercept to be at infinity for the special case where the plane is parallel to an axis.

Intercepts: α, β, γ

在分数坐标中指定截矩

➤ Step 2: Specify the intercepts in fractional co-ordinates.

Coordinates are converted to fractional coordinates by dividing the respective cell dimension. For example, a point (x, y, z) in a unit cell of dimensions $a \times b \times c$ has fractional coordinates of $(x/a, y/b, z/c)$. In the case of a cubic unit cell each coordinate will simply be divided by the cubic cell constant, a .

Fractional Intercepts: $\alpha/a, \beta/b$, and γ/c

➤ Step 3: Take the reciprocals of the fractional intercepts.

Miller Indices: (hkl)

取分数截矩的倒数

Crystallographic Notation

晶体学符号

- h, k and l are **all integers**;
- h, k and l are **co-prime**;
- Plane {110}:

 $(110)(\bar{1}10)(1\bar{1}0)(\bar{1}\bar{1}0)$

Notation	Interpretation
$(h k l)$	crystal plane
$\{h k l\}$	equivalent planes
$[h k l]$	crystal direction
$\langle h k l \rangle$	equivalent directions

- Direction $\langle 110 \rangle$:

 $[110][\bar{1}10][1\bar{1}0][\bar{1}\bar{1}0]$

h : inverse x-intercept of plane
 k : inverse y-intercept of plane
 l : inverse z-intercept of plane

等效面/等效方向：扩展晶体结构过程中，空间相对位置相同的面/方向