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

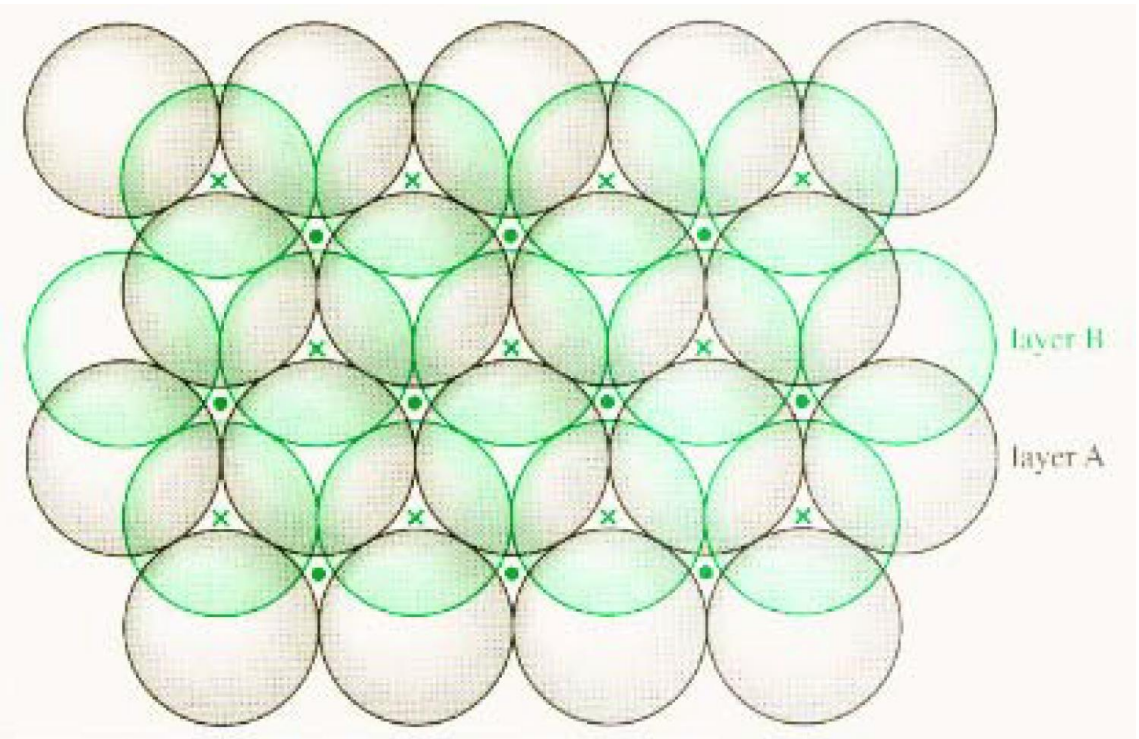
- To learn atomic packings in crystals;
- To understand **close packing**;
- To learn the typical crystal structures.

Atomic Packings (原子堆积)

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Packing (堆积)

- ❖ A crystal lattice can be described in terms of a packing of **non-overlapping rigid spheres**.
- ❖ Each type of atom in the crystal is considered as **spheres of identical size**.



Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Packing (堆积)

❖ The **tightness of packing** is determined by two factors:

I. **Packing Fraction** (**堆积比率，或堆积密度**): The fraction of volume in a crystal structure that is occupied by constituent particles.

$$\mathrm{PF} = \frac{N_{\mathrm{particle}} V_{\mathrm{particle}}}{V_{\mathrm{unit\ cell}}}$$

N_{particle}: The number of particles in the unit cell;

V_{particle}: The volume of each particle;

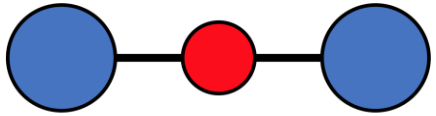
$V_{\mathrm{unit\ cell}}$: The volume occupied by the unit cell.

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

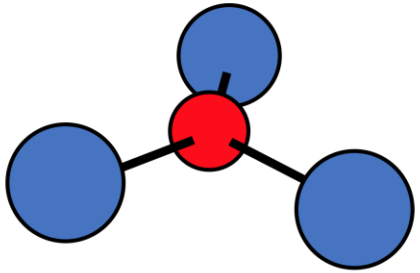
➢ Packing (堆积)

❖ The **tightness of packing** is determined by two factors:

II. **Coordination Number** (配位数): The number of atoms (or molecules/ions) bonded to a given atom (or molecule/ion) in a crystal.



CN = 2



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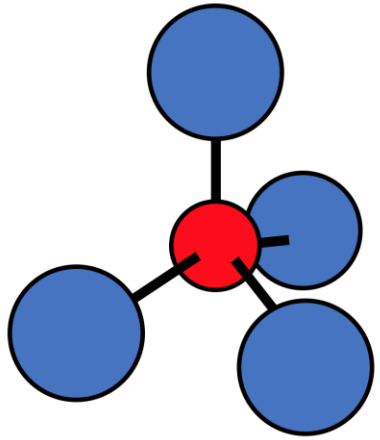
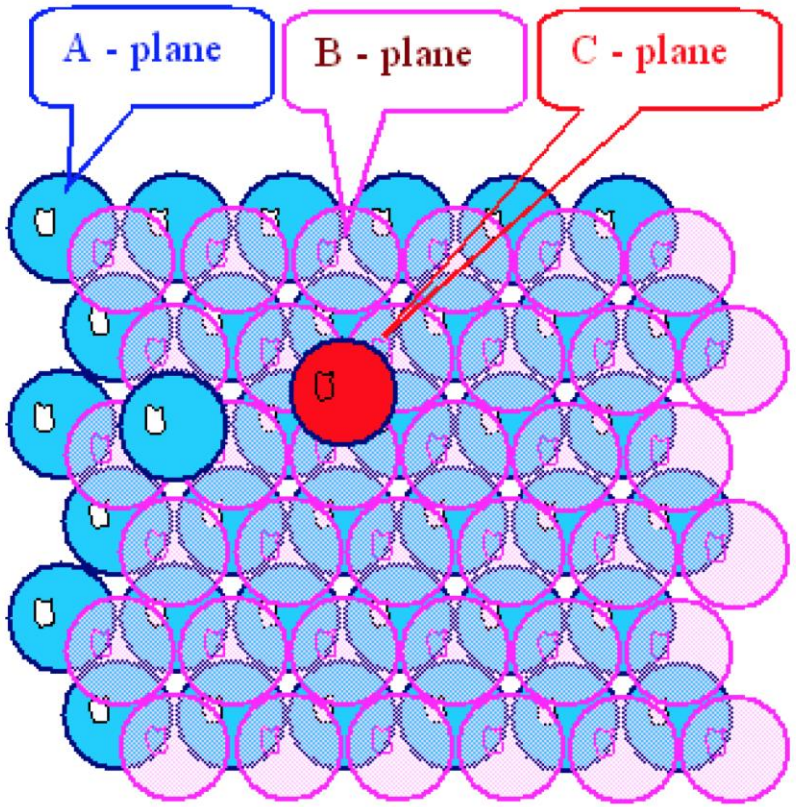


CN = 4

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Close Packing (密堆积)

❖ Close packing is a **dense arrangement** of equal spheres in a crystal lattice.

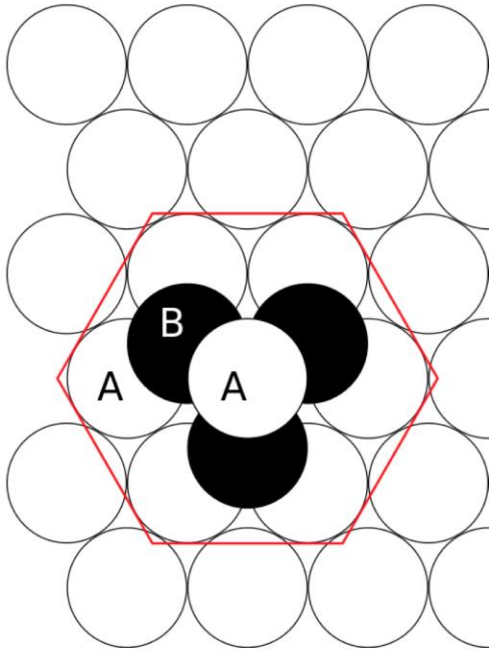


Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Close Packing (密堆积)

❖ There are **two close-packing structures** having denser packing than all other structures:

1) Hexagonal Close Packing (六角密堆, "HCP"):



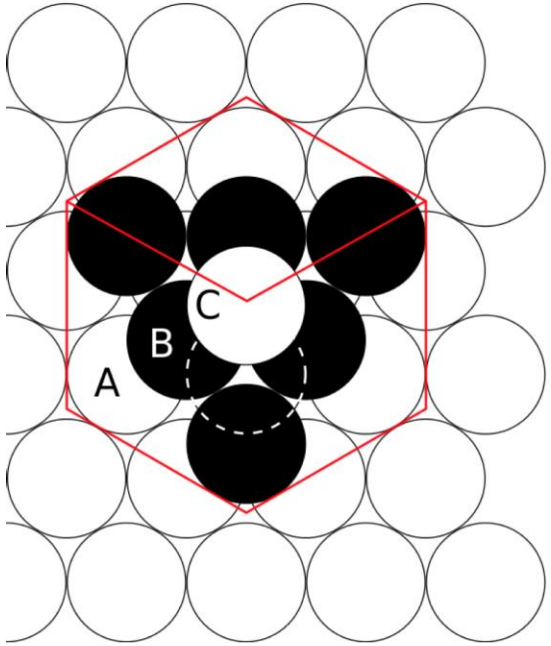
ABABAB….

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Close Packing (密堆积)

❖ There are **two close-packing structures** having denser packing than all other structures:

2) Cubic Close Packing (立方密堆, or Face-Centered Cubic, "FCC"):

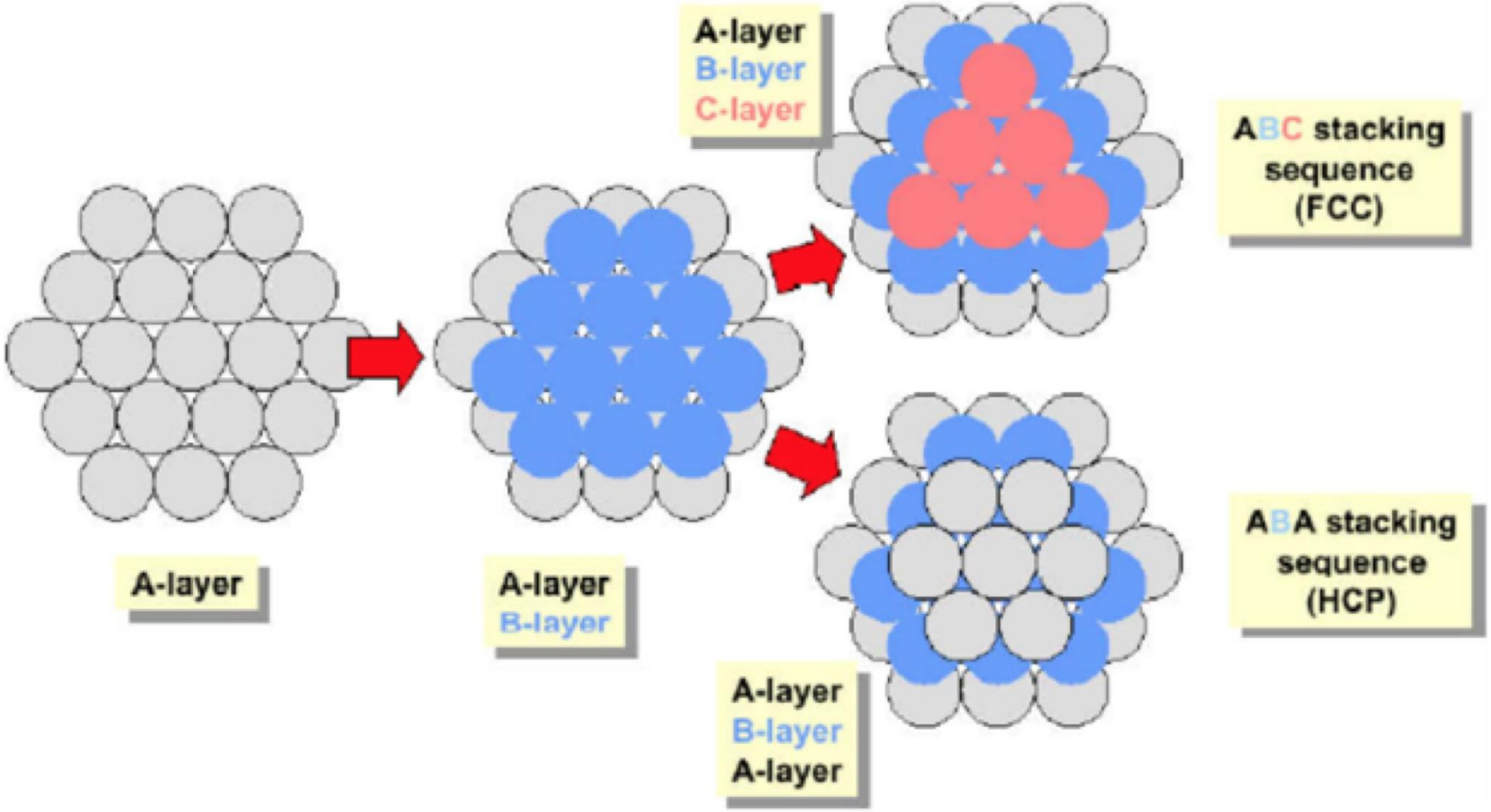


ABCABC….

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Close Packing (密堆积)

❖ There are **two close-packing structures** having denser packing than all other structures:



Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Close Packing (密堆积)

- ❖ The **coordination numbers** for HCP and FCC are both **12**.

- ❖ The **packing fractions** for HCP and FCC are also the highest:

$$\frac{\pi}{3\sqrt{2}} \simeq 0.74048$$

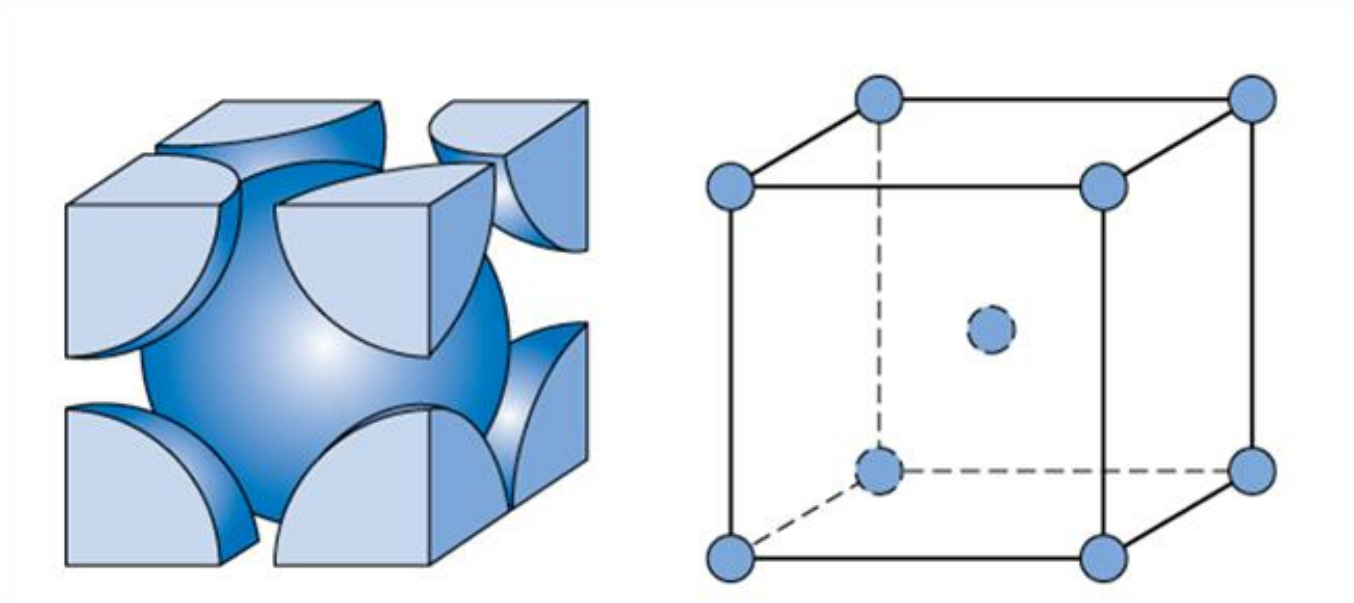
Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Other Packings

❖ Body-Centered Cubic (体心立方, **BCC**):

The packing fraction is **0.68**

The coordination number is **8**



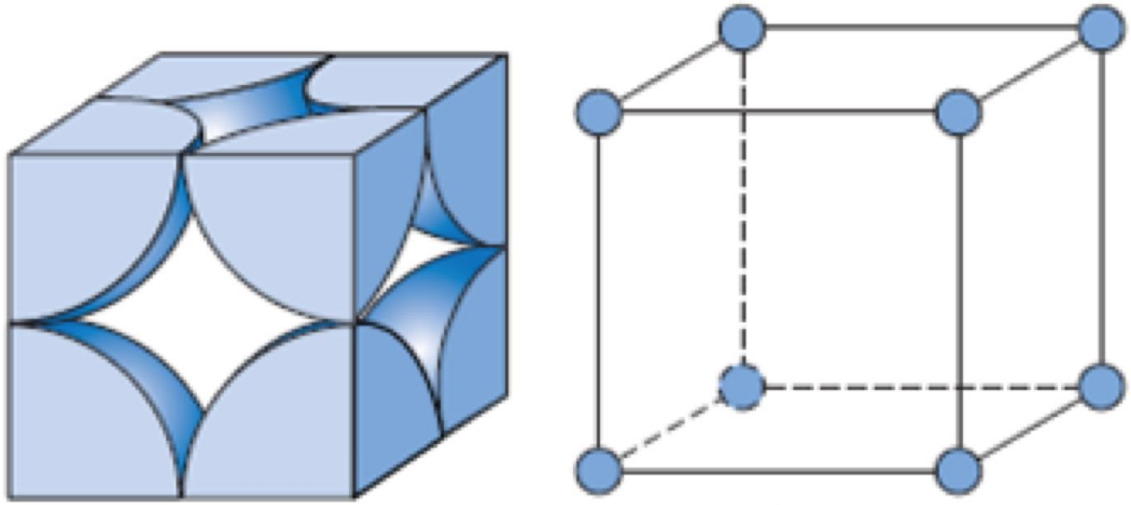
Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Other Packings

❖ Simple Cubic (简单立方, **SC**):

The packing fraction is **0.52**

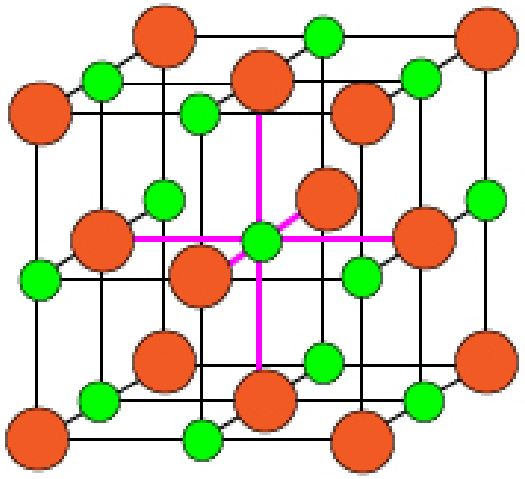
The coordination number is **6**

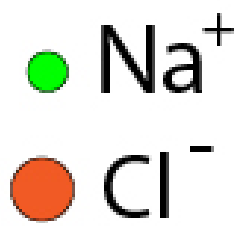


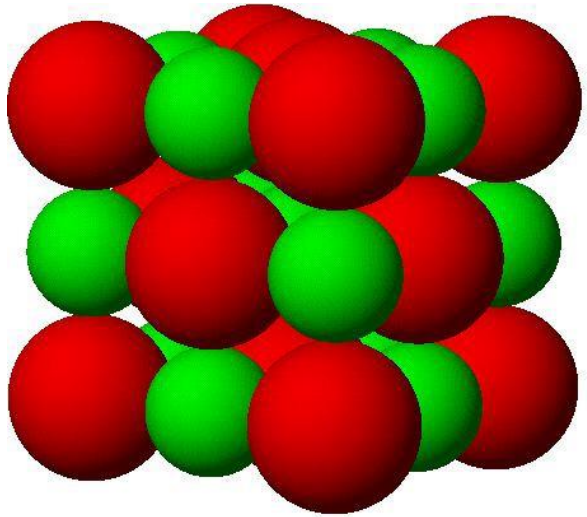
Examples of Crystal Structures (晶体结构实例)

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **NaCl Structure (NaCl型结构)**







Na^+	0 0 0	½ ½ 0	½ 0 ½	0 ½ ½
Cl^-	½ ½ ½	0 0 ½	0 ½ 0	½ 0 0

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ NaCl Structure (NaCl型结构)

- ❖ The lattice is **face-centered cubic (FCC);**
- ❖ The **basis** consists of one Na^+ ion and one Cl^- ion separated by one-half the body diagonal of a unit cell;
- ❖ Each ion has **6** nearest-neighbor ions of the opposite kind;
- ❖ There are **4** units of NaCl in each unit cell.

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

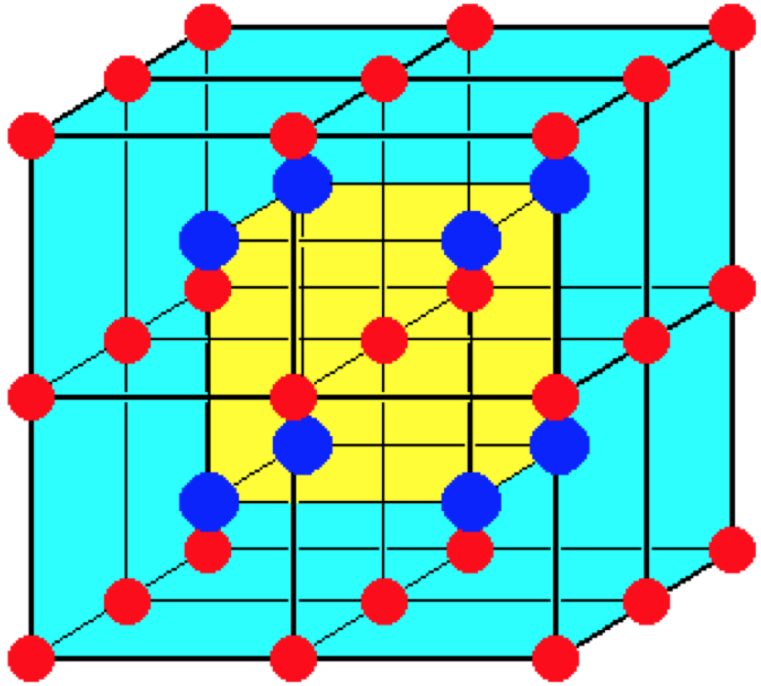
➢ NaCl Structure (NaCl型结构)

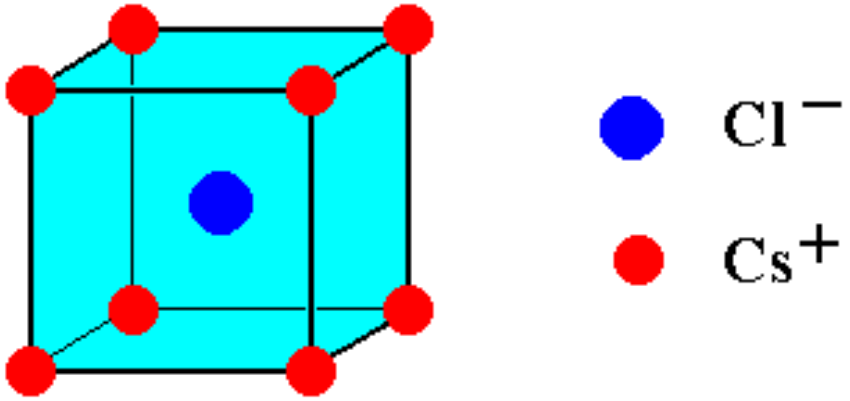
❖ Representative crystals having the NaCl structure include:

Crystal	a (Å)	Crystal	a (Å)
LiH	4.08	AgBr	5.77
MgO	4.20	PbS	5.92
MnO	4.43	KCl	6.29
NaCl	5.63	KBr	6.59

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **CsCl Structure (CsCl型结构)**





unit cell Cesium Chloride

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ CsCl Structure (CsCl型结构)

- ❖ The lattice is **simple cubic (SC);**
- ❖ There is **one CsCl "molecule" per unit cell** (primitive cell), with atoms at the corners (000) and body-centered positions (½ ½ ½) of the SC lattice;
- ❖ Each atom has **8** nearest-neighbor atoms of the opposite kind.

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ CsCl Structure (CsCl型结构)

❖ Representative crystals having the CsCl structure include:

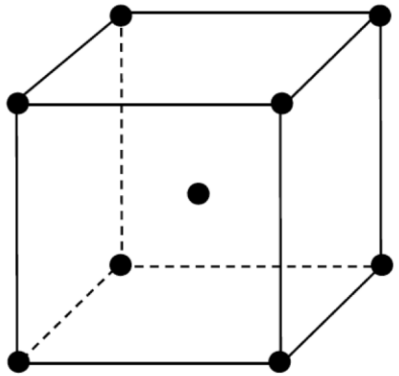
Crystal	a (Å)	Crystal	a (Å)
BeCu	2.70	LiHg	3.29
AlNi	2.88	NH_4Cl	3.87
CuZn (β-phase)	2.94	TlBr	3.97
CuPd	2.99	CsCl	4.11
AgMg	3.28	TlI	4.20

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

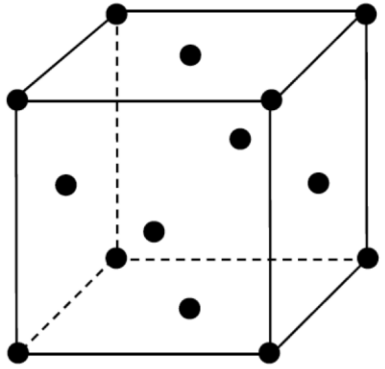
➢ Simple Lattice VS Compound Lattice (简单晶格Vs复式晶格)

❖ Simple lattice (简单晶格):

- There is only **one atom per primitive cell (or basis)**;
- **All atoms are identical** in terms of their chemical properties, positions in the lattice, and coordination numbers.



BCC simple lattice



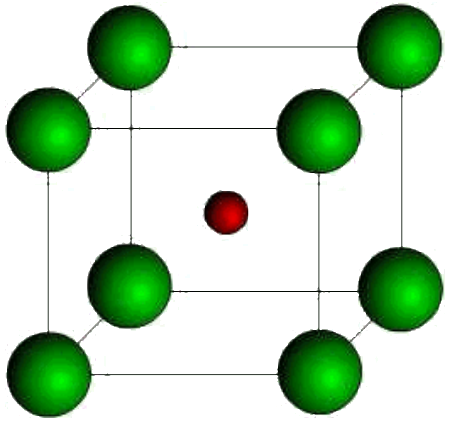
FCC simple lattice

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

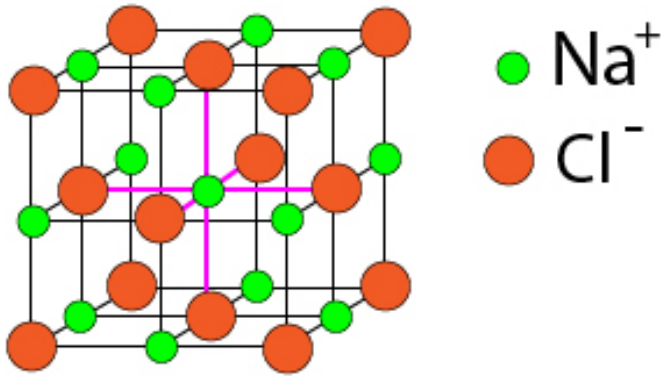
➢ Simple Lattice VS Compound Lattice (简单晶格Vs复式晶格)

❖ Compound lattice (复式晶格):

- There are **more than one atoms per primitive cell (or basis)**;
- The atoms in a cell (or basis) can be of **the same type or different types**.
- The corresponding atoms of different cells form **the same type of simple lattice**.



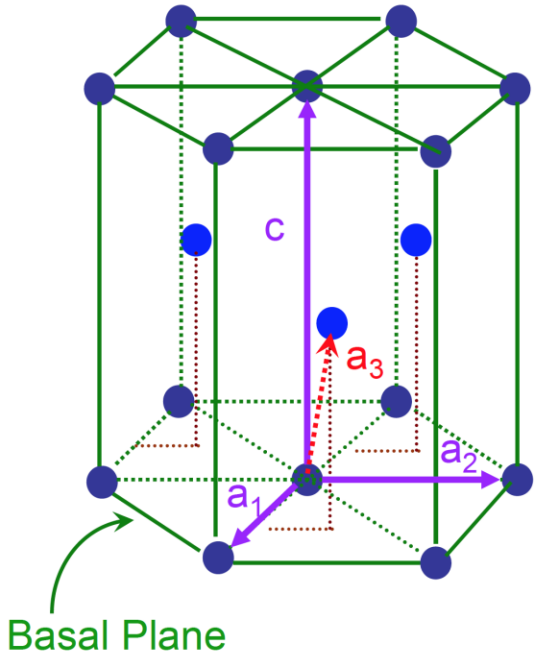
SC compound lattice

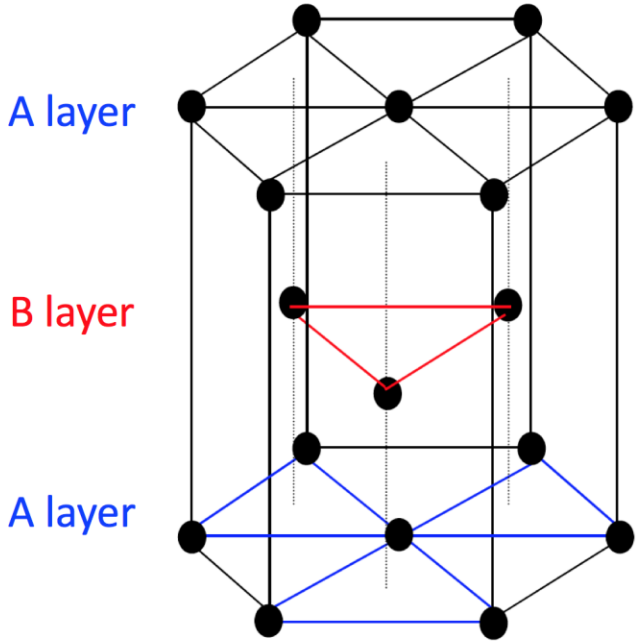


FCC compound lattice

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **HCP Structure (六角密堆积型结构)**





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Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ HCP Structure (六角密堆积型结构)

- ❖ The primitive cell has a_1=a_2, with an angle of 120°;
- ❖ The c axis is normal to the plane of a_1 and a_2;
- ❖ The ideal HCP structure has ***c* = 1.633 *a***;
- ❖ One basis has **2** atoms, with one at (000) and the other at (2/3 1/3 1/2).

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

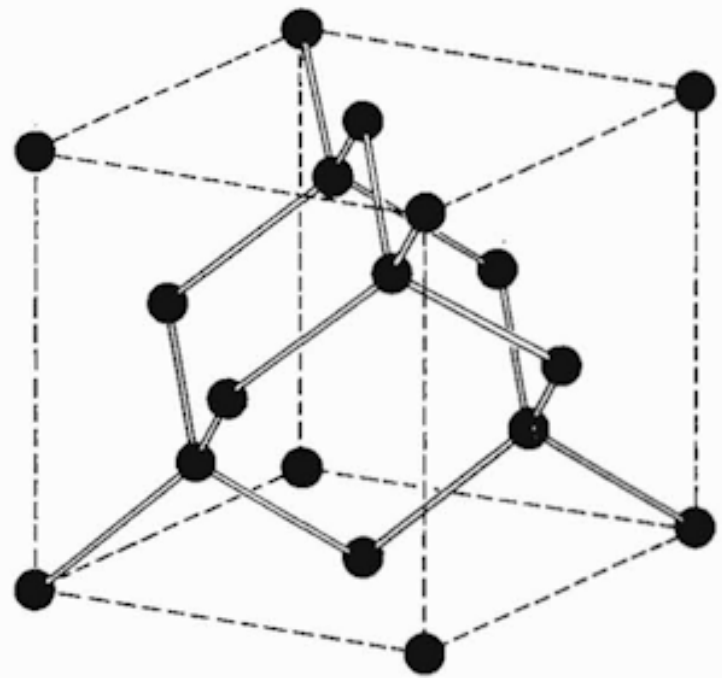
➢ HCP Structure (六角密堆积型结构)

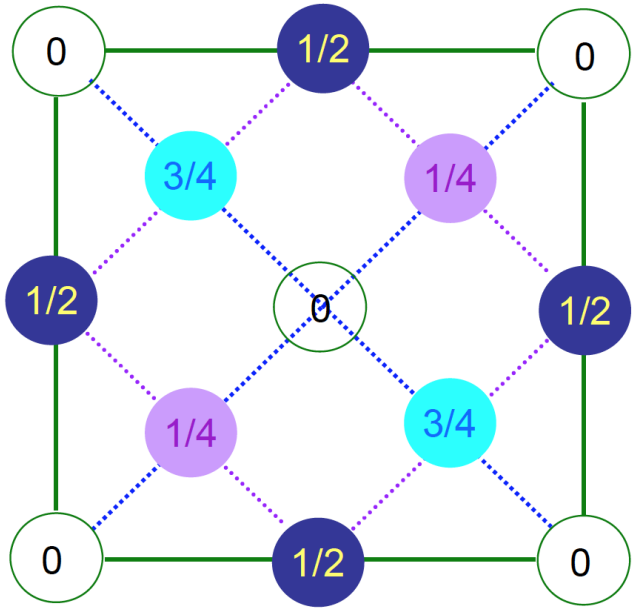
❖ Representative crystals having the HCP structure include:

Crystal	c/a	Crystal	c/a
He	1.633	Co	1.622
Be	1.581	Y	1.570
Mg	1.623	Zr	1.594
Ti	1.586	Gd	1.592
Zn	1.861	Lu	1.586
Cd	1.886		

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **Diamond Structure (金刚石型结构)**





Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Diamond Structure (金刚石型结构)

- ❖ The lattice is **face-centered cubic (FCC);**
- ❖ The primitive basis has **2 identical atoms** at coordinates (000) and (¼ ¼ ¼);
- ❖ Because the unit cell of FCC contains **4 lattice sites**, the unit cell of the diamond structure contains 2×4=**8 atoms**;
- ❖ The packing fraction is only **0.34** (46% of the FCC packing).

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

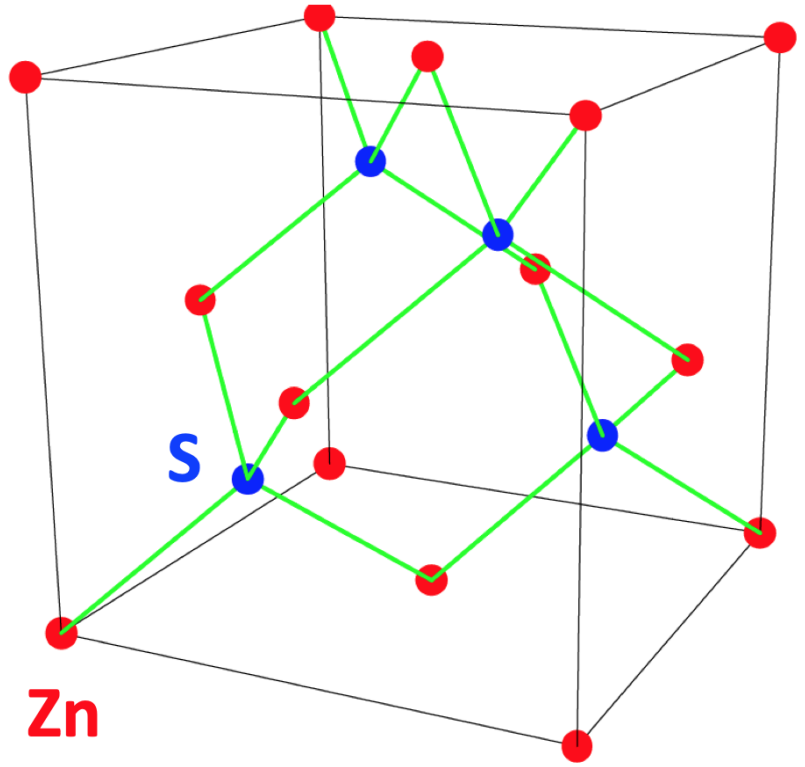
➢ Diamond Structure (金刚石型结构)

❖ Representative crystals having the diamond structure include:

Crystal	a (Å)	Crystal	a (Å)
C (diamond)	3.576	Ge	5.658
Si	5.430	Sn	6.49

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **Cubic ZnS Structure (立方硫化锌型结构)**



Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Cubic ZnS Structure (立方硫化锌型结构)

- ❖ The Cubic ZnS (**Zinc Blende 闪锌矿**) structure is similar to the diamond (FCC) structure.
- ❖ The Zn atoms are placed on one FCC lattice and the S atoms on the other FCC lattice.
- ❖ There are **4 "molecules" of ZnS per unit cell**.
- ❖ Each atom has 4 equally distant atoms of the opposite kind.
- ❖ The ZnS structure **does NOT have inversion symmetry** (while the diamond structure does have).

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

- **Cubic ZnS Structure (立方硫化锌型结构)**

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雷伟杰 王嘉谦 赵源祥
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Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Cubic ZnS Structure (立方硫化锌型结构)

❖ Representative crystals having the cubic ZnS structure include:

Crystal	a (Å)	Crystal	a (Å)
SiC	4.35	ZnSe	5.65
ZnS	5.41	GaAs	5.65
AlP	5.45	AlAs	5.66
GaP	5.45	InSb	6.46

Summary (总结)

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

➢ Summary (总结)

❖ Atomic Packing in Crystals:

1) HCP (close packing) **2) FCC (close packing)**

3) BCC 4) SC

❖ Typical Crystal Structures:

1) NaCl 2) CsCl 3) HCP 4) Diamond

5) Cubic ZnS

Chapter 1.3: 课后作业

如果将等体积球分别排列成下列结构, 计算出钢球所占体积与总体积之比:

1) 简单立方, 2) 体心立方, 3) 面心立方, 4) 六角密堆, 5) 金刚石结构

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