Chapter 1

Crystal Structure
(晶体结构)

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)

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- **Chapter 1.4** Reciprocal Lattice (倒易点阵)

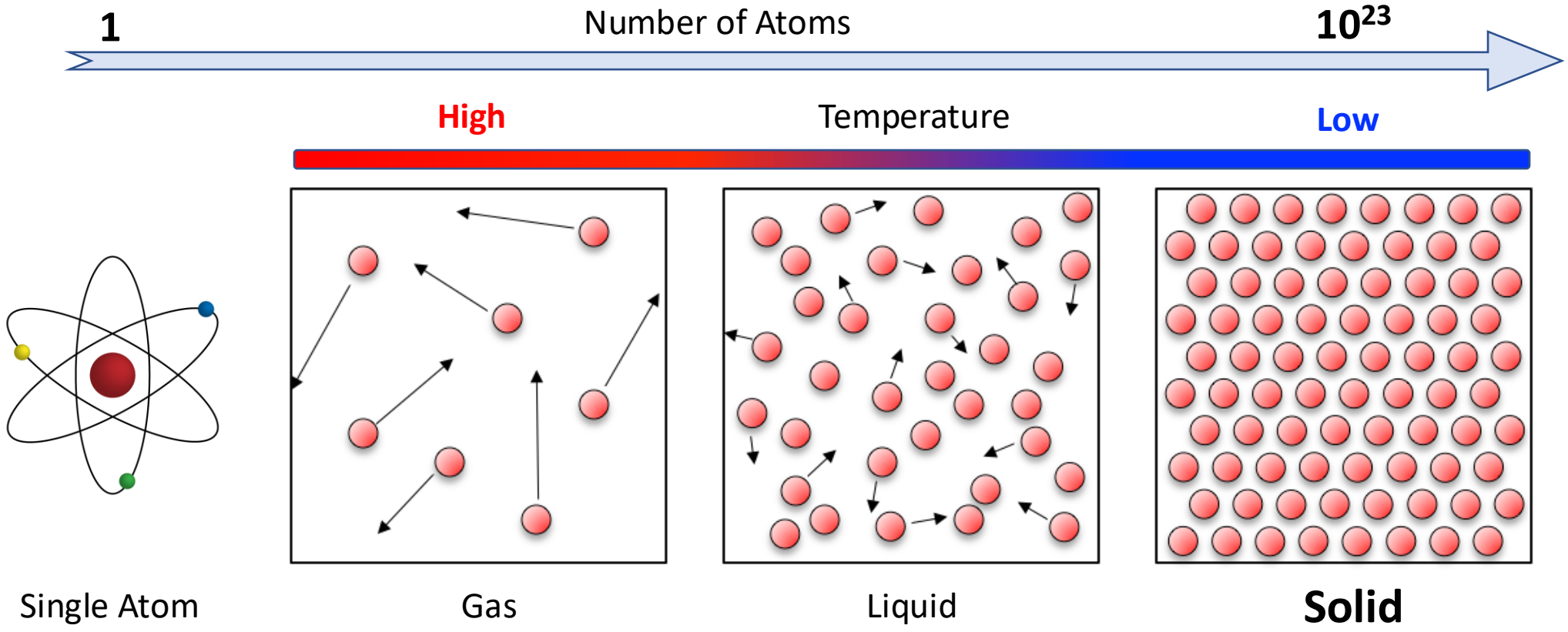
Objectives

- To learn the classification of solid materials;
- To understand the concept of “**crystal lattice**” and its properties.

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Solid (固体)

- ❖ Solid is one of the four **fundamental states of matter** (gas, liquid, solid, and plasma).
- ❖ A solid material has **definite shape and volume**.



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

- **Examples of Solid Materials**

Gold (Au)

Diamond (C)

Quartz (SiO_2)

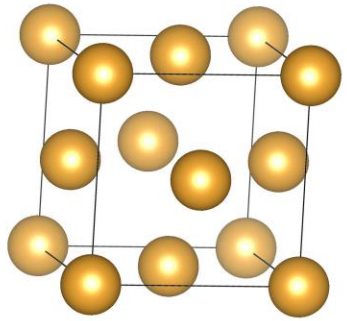
Salt (NaCl)

Polymer

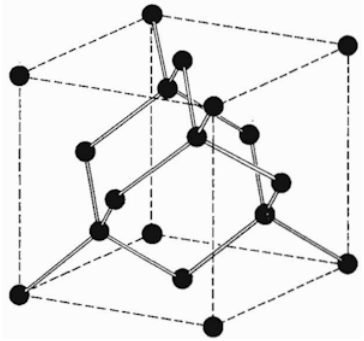
Glass

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

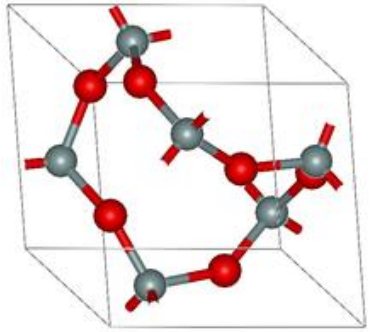
➢ Microscopic Structures of Solid Materials



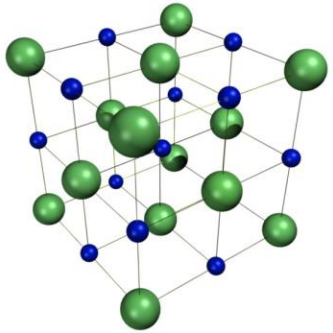
Gold (Au)



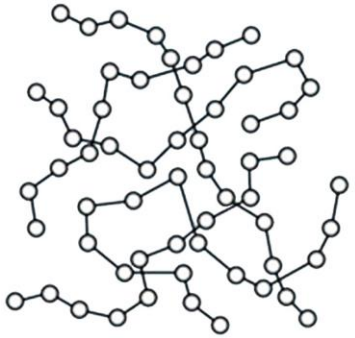
Diamond (C)



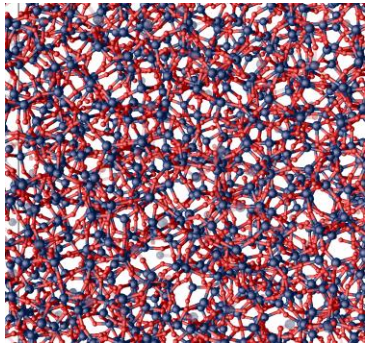
Quartz (SiO_2)



Salt (NaCl)



Polymer



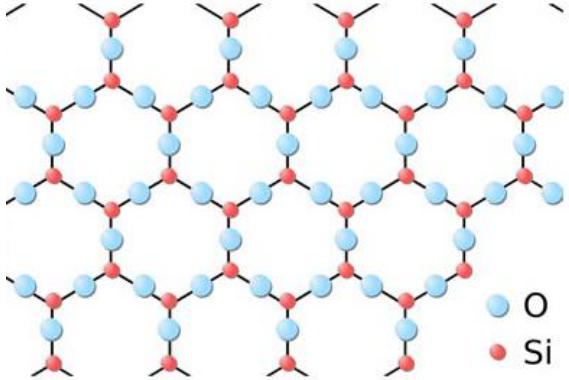
Glass

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

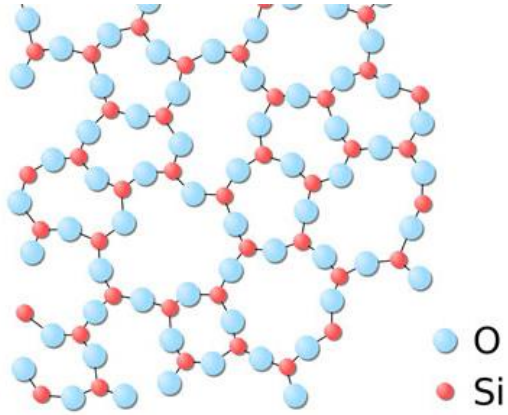
➢ Classifications of Solid Materials

Solid Materials

- **Crystals (晶体)**
- **Noncrystals (非晶体)**



Quartz (SiO_2)



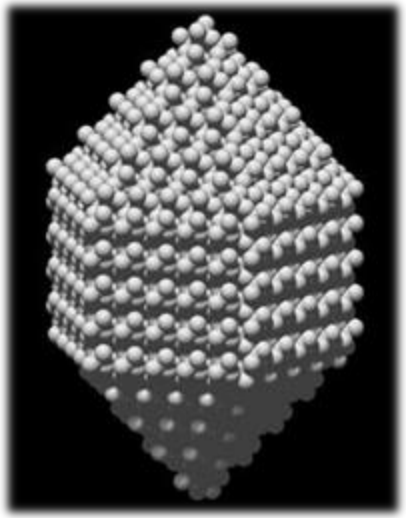
Glass (mostly SiO_2)

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Crystals

- ❖ Crystals are built of a **periodic array of atoms (or groups of atoms)**;
- ❖ A crystal has a **regular shape** and **both macroscopic and microscopic symmetries**;
- ❖ A crystal has a fixed melting point.
- ❖ A crystal can split along definite structural planes (cleavage).
- ❖ The crystal properties are anisotropic (各向异性).

Quartz Crystal



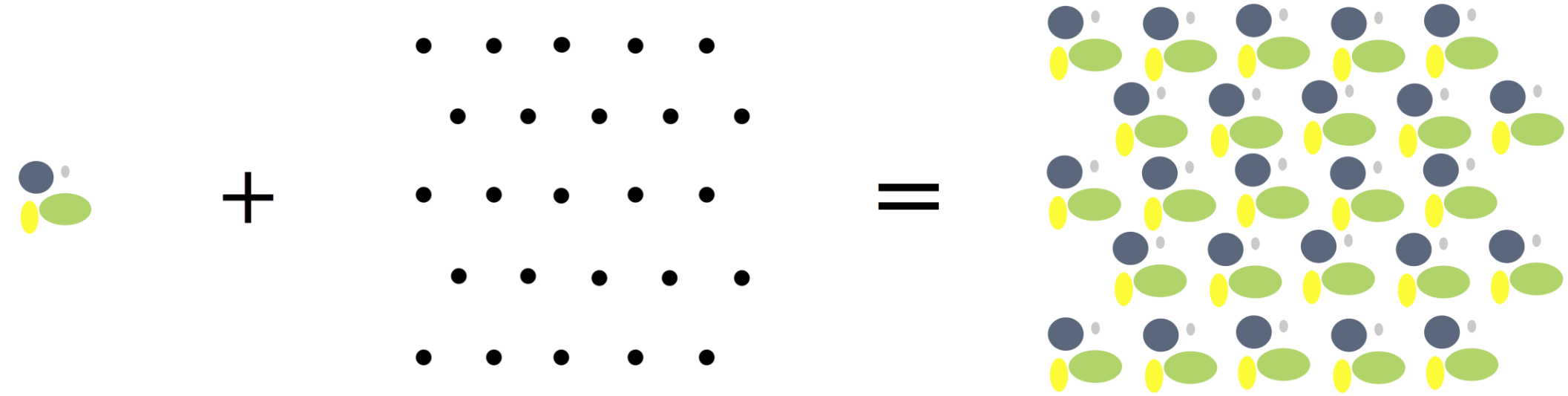
Idealized Quartz Crystal

Cleavage (解理)

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Crystal Lattice (晶格)

- ❖ An ideal crystal is constructed by the **infinite repetition of identical atoms or groups of atoms**.
- ❖ A group is called the **basis (基元)**.
- ❖ The set of mathematical points to which the basis is attached is called the **crystal lattice (晶格)**.

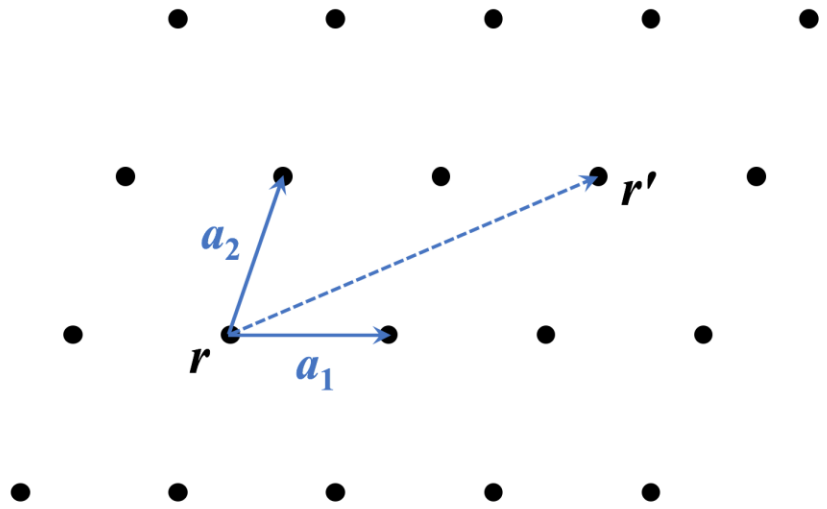


Basis **Lattice** **Crystal**

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Lattice Translation Vectors (晶格平移矢量)

- ❖ The lattice can be defined by a set of **translation vectors** $\boldsymbol{a_i}$
- ❖ The arrangement of atoms in the crystal looks the same when viewed from the site $\boldsymbol{r}$ as when viewed from every site $\boldsymbol{r'}$ translated by an integral multiple of the $\boldsymbol{a_i}$.



Three-Dimensional (3D):

$$\boldsymbol{r' = r + u_1 a_1 + u_2 a_2 + u_3 a_3}$$

Two-Dimensional (2D):

$$\boldsymbol{r' = r + u_1 a_1 + u_2 a_2}$$

One-Dimensional (1D):

$$\boldsymbol{r' = r + u_1 a_1}$$

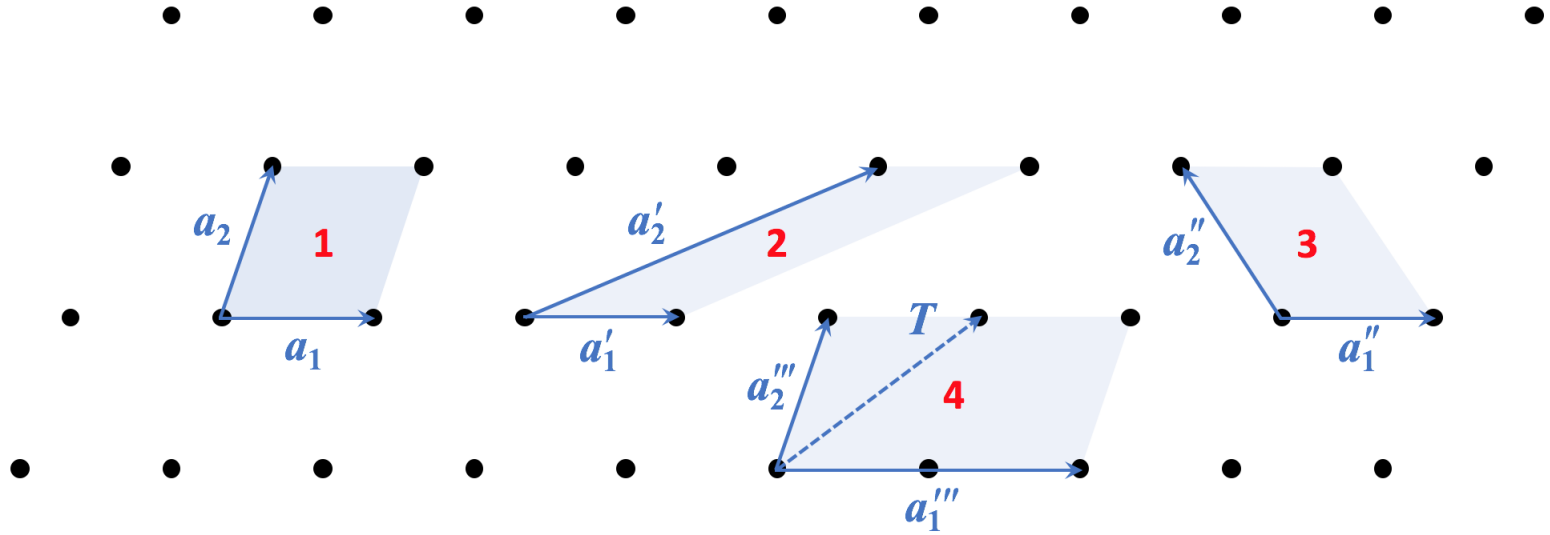
Here, $\boldsymbol{u_i}$ are arbitrary integers.
The set of sites $\boldsymbol{r'}$ defined by the above equations for all $\boldsymbol{u_i}$ defines the lattice.

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Primitive Translation Vectors (初基平移矢量)

❖ The primitive translation vectors (**primitive vectors**) $\boldsymbol{a_i}$ are such that there is no cell of volume smaller than $\boldsymbol{a_1 \cdot a_2 \times a_3}$ that can serve as a building block for the crystal structure.

❖ The primitive vectors are often used to define the **crystal axes (晶轴)**.

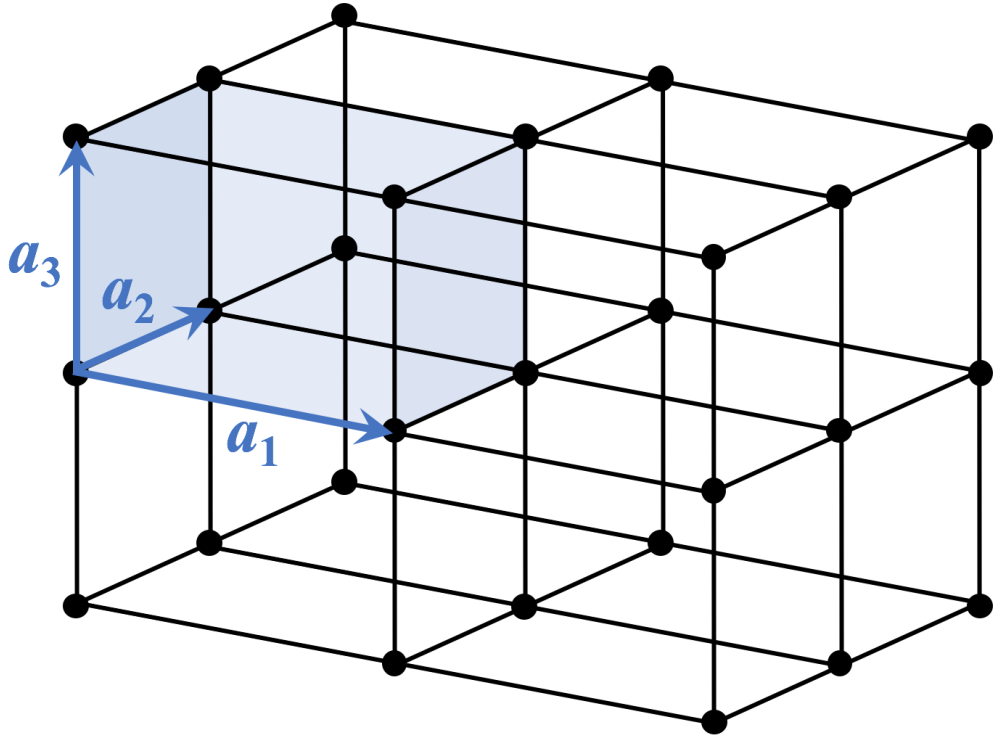


*The vectors in 4 are not primitive because the lattice translation *T* cannot be formed from integral combinations of these vectors.

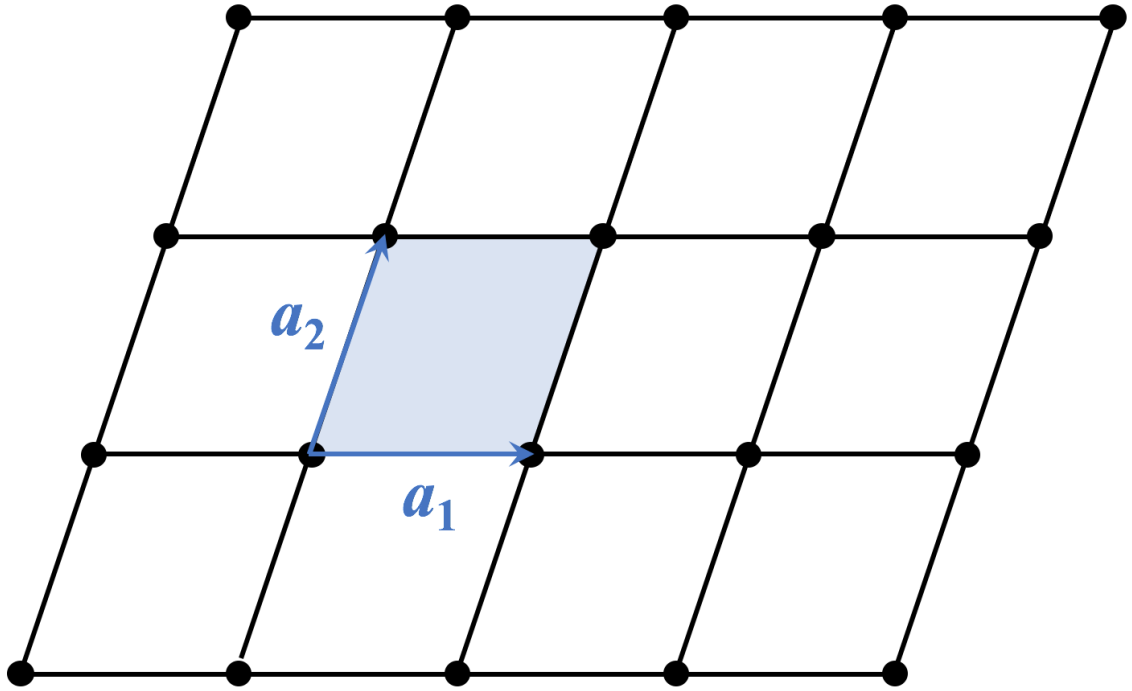
Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Primitive Cell (原胞)

❖ A primitive cell is the **parallelepiped** (or **parallelogram** in 2D) defined by primitive vectors a_i.



3D



2D

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Primitive Cell (原胞)

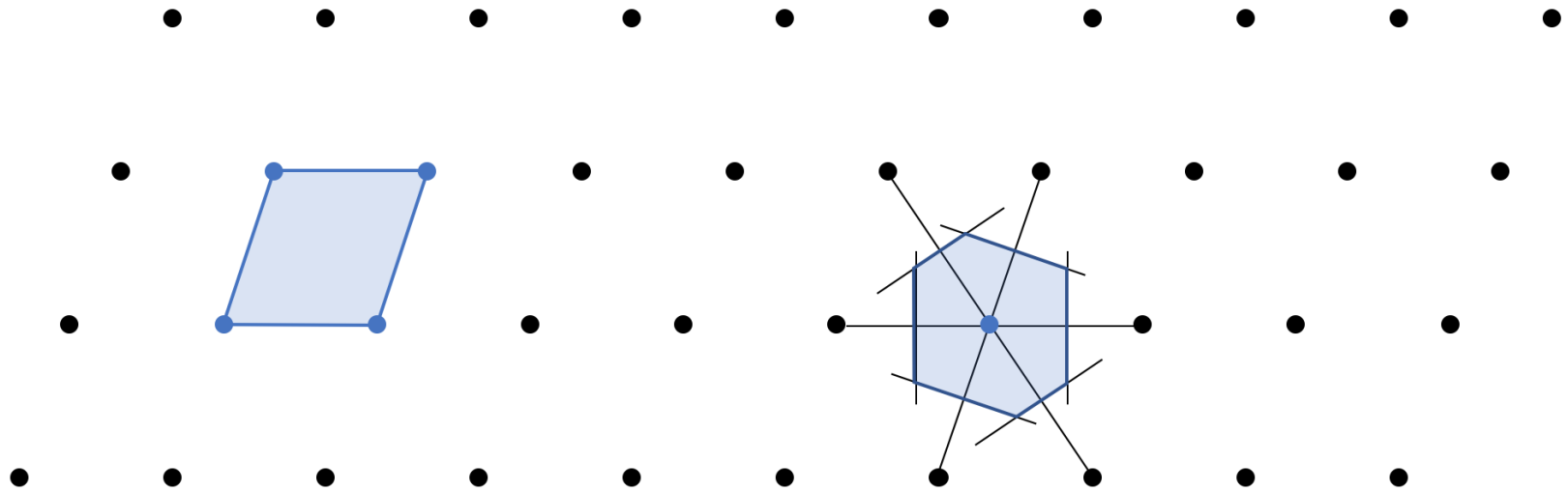
- ❖ A primitive cell is a **building block** of the crystal structure;
- ❖ A primitive cell will fill all space by the repetition of suitable crystal **translation operations**;
- ❖ A primitive cell is a **minimum-volume cell ($\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3$);**
- ❖ There is **only one lattice site (not atoms) per primitive cell**;
- ❖ There are many ways of choosing the primitive vectors and primitive cell for a given lattice;
- ❖ The number of atoms in a primitive cell is always the same for a given crystal structure.

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Wigner-Seitz Cell (维格纳-赛茨原胞)

❖ Wigner-Seitz cell is **a special type of primitive cell** and it can be chosen by following this procedure:

1. Draw lines to connect a given lattice site to all nearby lattice sites;
2. At the midpoint and normal to these lines, draw new lines or planes;
3. The **smallest volume enclosed in this way** is the Wigner-Seitz cell.

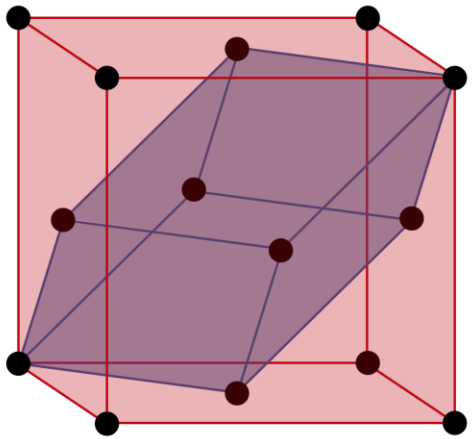


Regular Primitive Cell **Wigner-Seitz Cell**

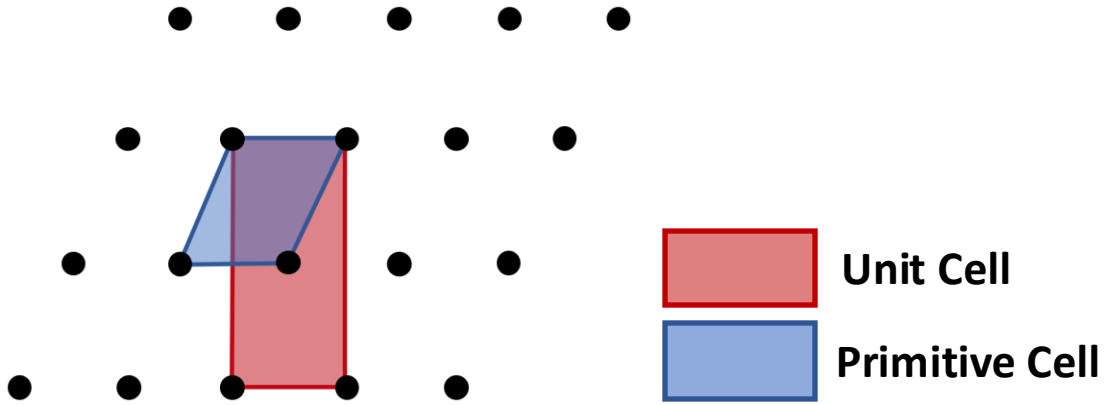
Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Unit Cell (单胞)

- ❖ A unit cell (also called **conventional cell**) is defined as **the smallest repeating unit having the full symmetry of the crystal structure**;
- ❖ A unit cell is also a **building block** of the crystal structure;
- ❖ For a given lattice, the volume (or area in 2D) of the unit cell is always **an integral multiple** of that of the primitive cell.



3D



2D

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

- **Unit Cell (单胞)**

Properties	Unit Cell	Primitive Cell
Have Symmetry of the Crystal Structure	Full Symmetry	Only Translational Symmetry
Impartible Repeating Unit?	Yes	Yes
Minimum-Volume Cell?	Not Necessary	Yes
Number of Lattice Points per Cell	≥ 1	1

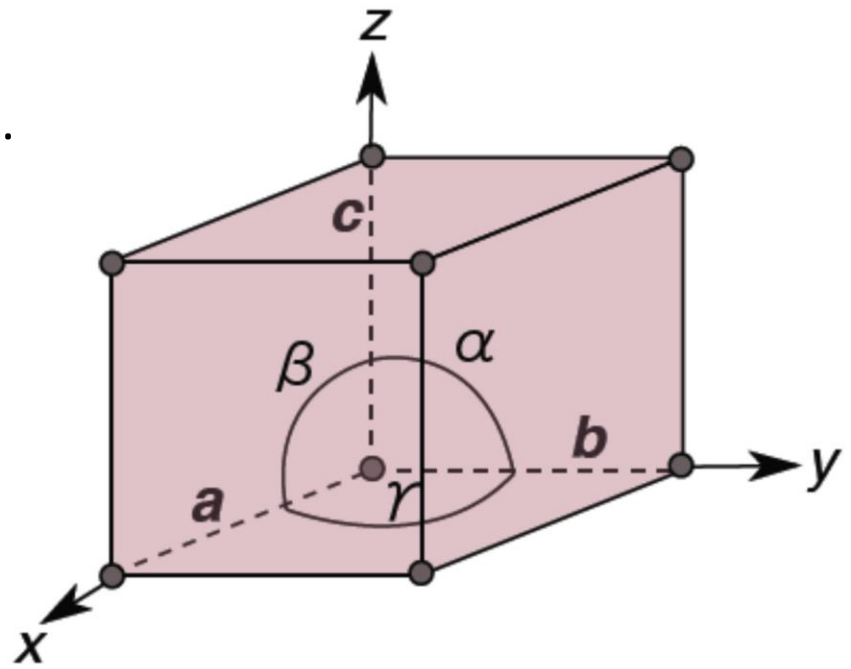
Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Lattice Parameters (晶胞参数)

- ❖ To define the geometry of the **unit cell** in 3D, we choose a right-handed set of crystallographic axes, x, y, and z, which point along the edges of the unit cell;
- ❖ The origin of the coordinate system is at one of the lattice sites;
- ❖ The lengths of the unit cell along the x, y, and z direction are defined as $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$, also called lattice constant.
- ❖ The angles between $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$, are defined as α, β, and γ.

$$\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}, \alpha, \beta, \gamma$$

α = the angle between $\boldsymbol{b}$ and $\boldsymbol{c}$
β = the angle between $\boldsymbol{a}$ and $\boldsymbol{c}$
γ = the angle between $\boldsymbol{a}$ and $\boldsymbol{b}$



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Lattice Parameters (晶胞参数)

An Example: **SiO_2**

$a = 4.913$ Å

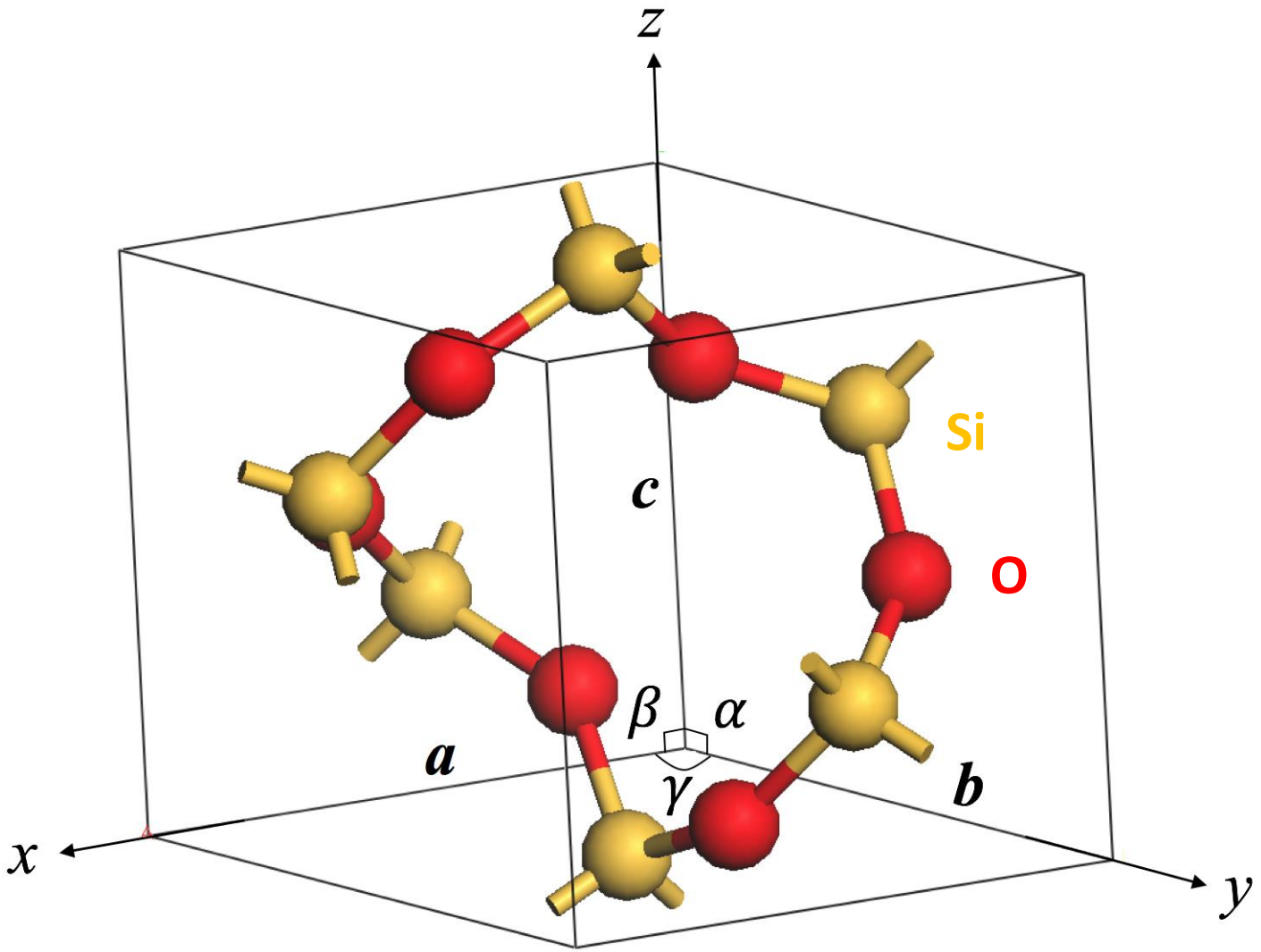
$b = 4.913$ Å

$c = 5.405$ Å

$\alpha = 90°$

$\beta = 90°$

$\gamma = 120°$



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

❖ The orientation of a crystal plane can be specified by the indices determined by the following rules:

1) Find the intercepts (截距) on the axes in terms of the lattice constants a_1, a_2, a_3. The axes may be those of a primitive or non-primitive cell.

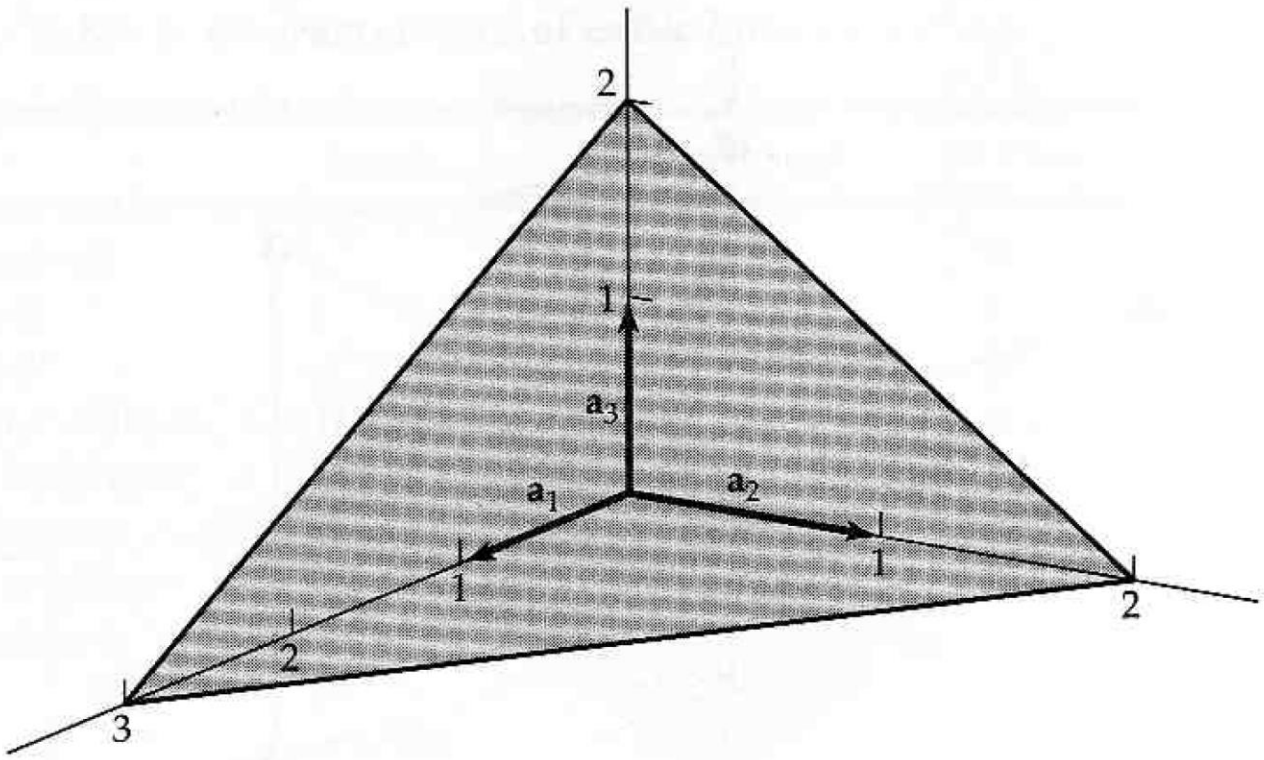
2) Take the reciprocals of these numbers (i.e., the intercepts) and then reduce to three integers having the same ratio, usually the smallest three integers.

3) The result, enclosed in parentheses (hkl), is called the index of the plane (晶面指数)

❖ The index obtained in this way is also called **Miller Index** (密勒指数).

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)



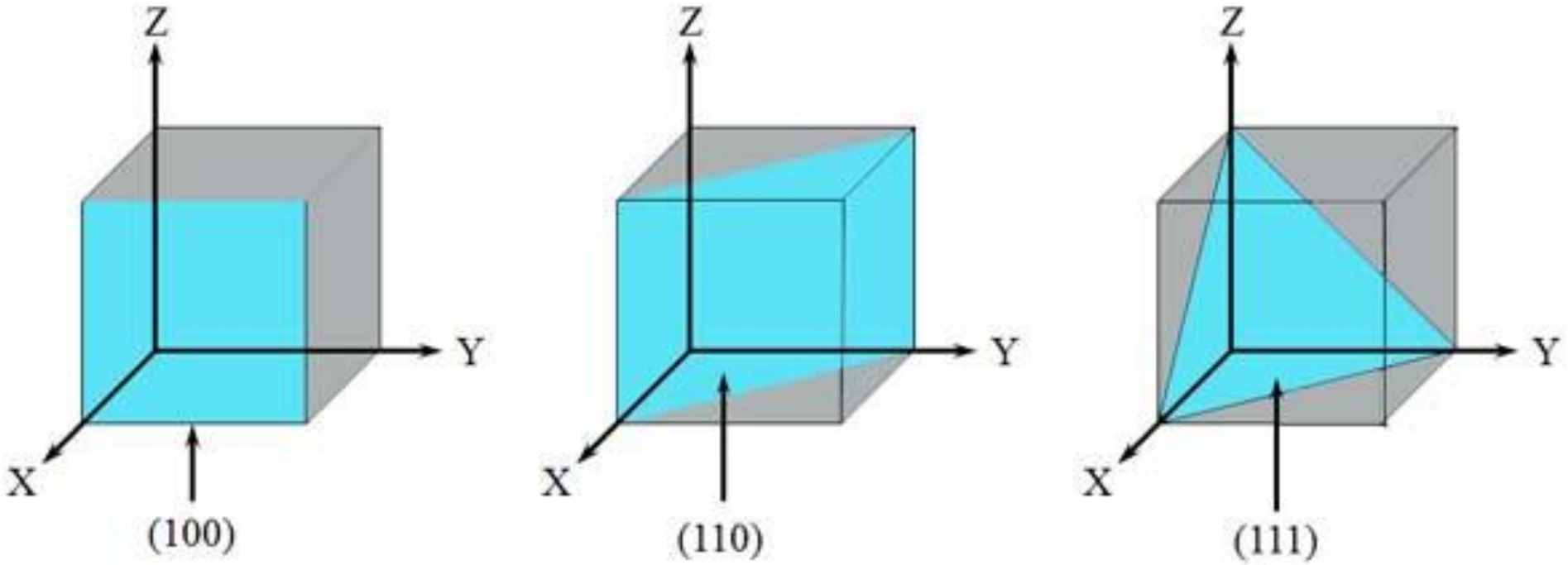
This plane intercepts the a_1, a_2, a_3 axes at $3a_1$, $2a_2$, $2a_3$. The reciprocals of these numbers are 1/3, 1/2, 1/2.

The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

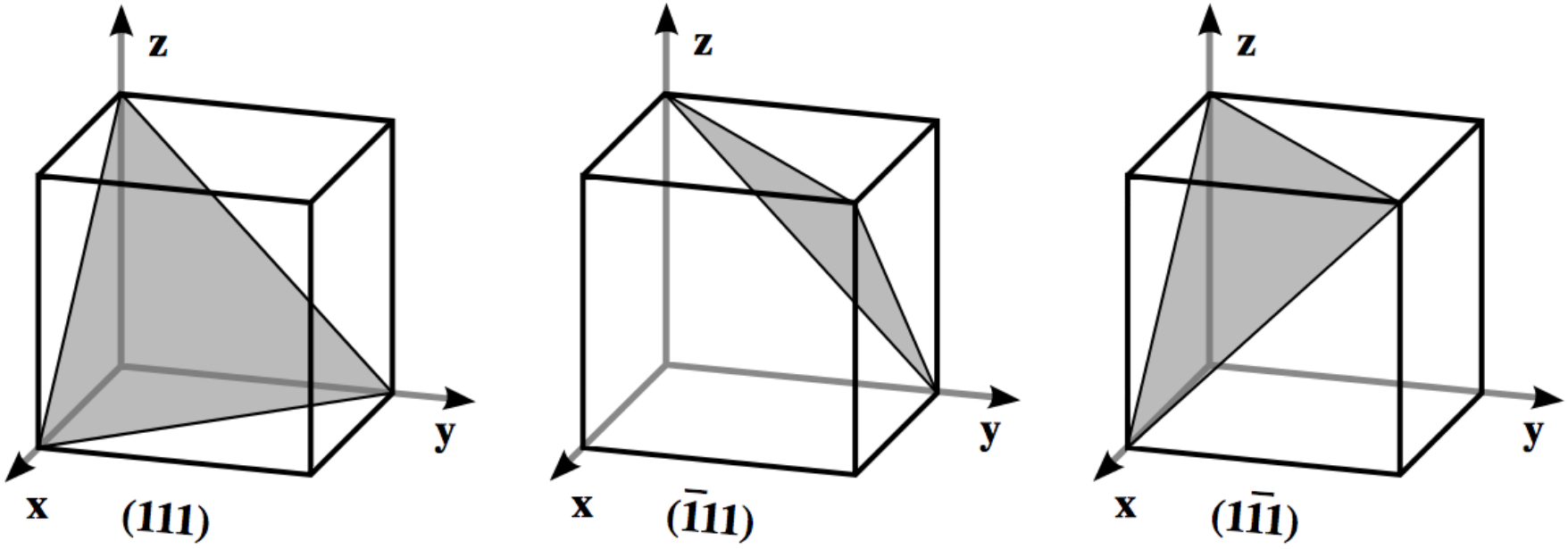
- ❖ For an intercept at infinity, the corresponding index is zero.
- ❖ The indices (*hkl*) may denote a single plane or a set of parallel planes.



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

❖ If a plane cuts an axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index, e.g., $(h\bar{k}l)$.

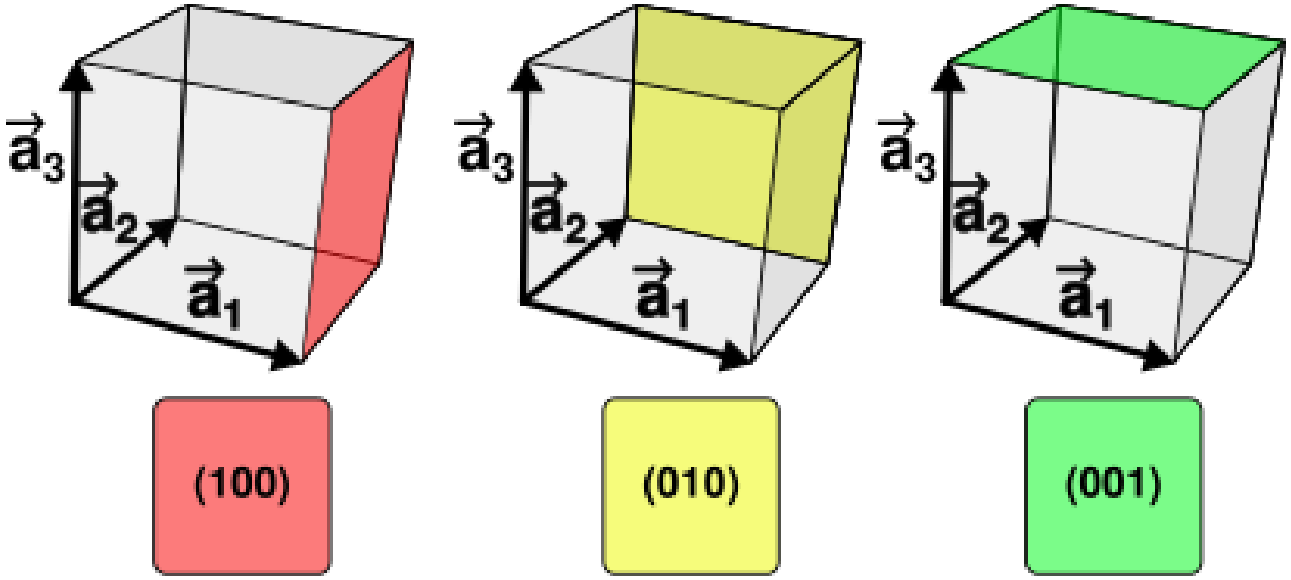


Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

❖ Planes equivalent by symmetry may be denoted by curly brackets around indices, i.e., $\{hkl\}$.

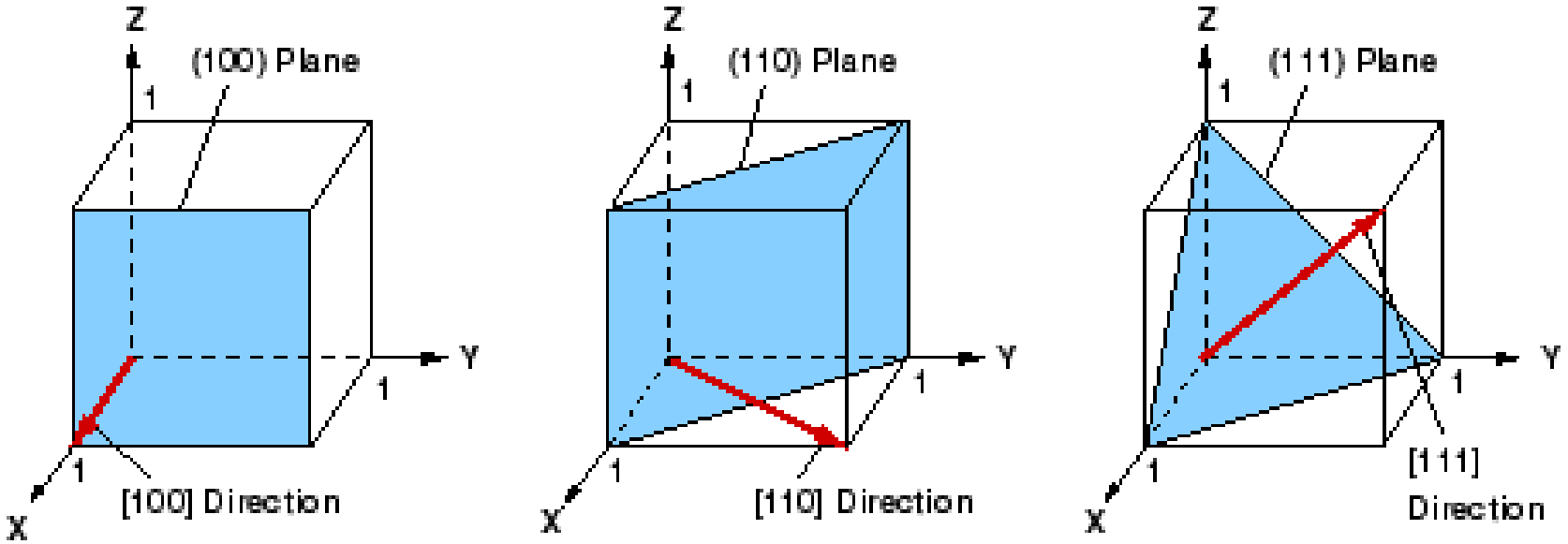
The following set of cube faces is {100}.



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

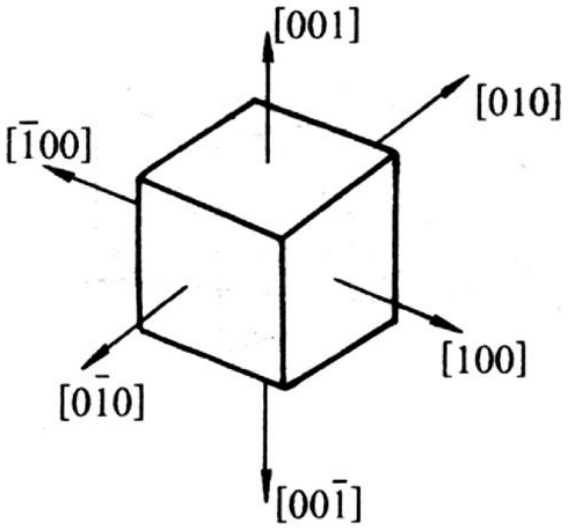
- ❖ [*hkl*] denotes a crystal direction (晶向) on the basis of the lattice vectors.
- ❖ In cubic crystals, the direction [*hkl*] is perpendicular to a plane (*hkl*) having the same indices, but this is not generally true in other crystal systems.



Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Index System for Crystal Planes (晶面指数系统)

❖ The notation <*hkl*> denotes the set of all directions that are equivalent to [*hkl*] by symmetry.



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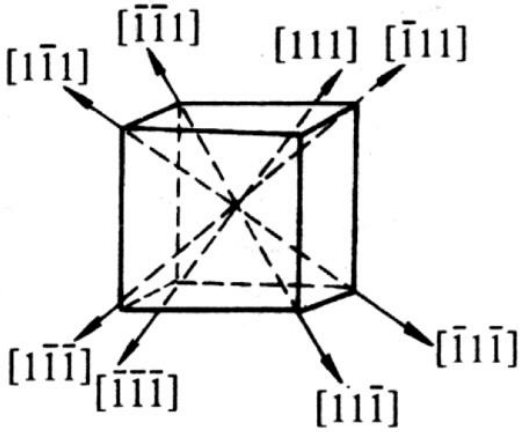

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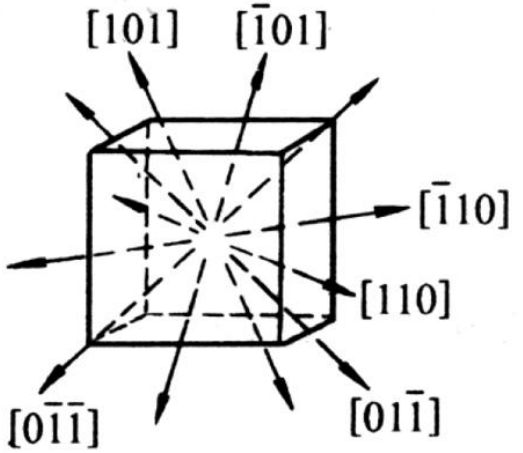

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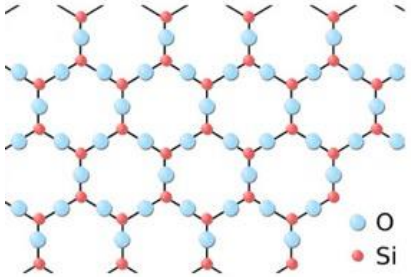
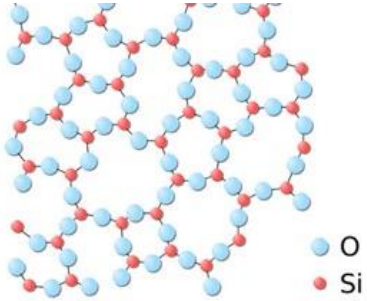
Summary (总结)

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

➢ Summary (总结)

❖ Solid Materials:

1) Crystals 

2) Noncrystals 

❖ Crystal Lattice: Basis (基元) + Lattice (格点)

❖ Properties of Crystal Lattice:

1) Translation vectors; 2) Primitive cell; 3) Unit cell; 4) Miller Index

Chapter 1.1: 课后作业

1. 分别画出硅(silicon)晶体的一个单胞(unit cell)和一个原胞(primitive cell)，并分别指出其各自含有的硅原子数目。
2. 分别画出硅晶体(100)、(110)和(111)面上的原子排列。

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